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VAPOR PRESSURE DATA ANALYSIS METHODOLOGY, STATISTICS, AND APPLICATIONS

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RESEARCH DIRECTORATE

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A method of fitting vapor pressure temperature data to the Antoine equation is described along with a detailed statistical analysis of the fits and calculations of vapor pressures, enthalpies of vaporization, volatilities (concentration of saturated vapors), and boiling points with the Antoine constants. It is shown that the number of digits required to accurately perform vapor pressure calculations is greater than previously believed. The system permits calculation of the limits of error for any level of confidence. A program is used to analyze and plot the available vapor pressure data for diethyl malonate.

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PREFACE

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VAPOR PRESSURE DATA ANALYSIS METHODOLOGY, STATISTICS, AND APPLICATIONS

1. INTRODUCTION

Vapor pressure is one of the most important liquid properties. Vapor pressures have a strong influence on the volatility, reactivity, persistency, toxicity, flammability, solubility, and transfer processes of chemicals. It is a strong function of temperature - increasing from 20 to 1000 % every ten degrees Celsius. For that reason it is usually plotted against temperature on a logarithmic scale. The slope of a plot of vapor pressures versus temperatures is used to calculate the enthalpy of vaporization which is used to calculate other thermodynamic properties. For such reasons a very precise knowledge of vapor pressures is required for both basic research and practical applications.

Many of the vapor pressure equations or values found in the literature or commercial computerized data bases need to be re-evaluated. Errors run as high as several hundred percent and careful statistical analysis is required.

Decontamination is a typical example of the application of vapor pressure data. In many hazardous chemical situations, there are probably few alternatives other than relying on natural decontamination. Calculations hazardous chemical persistence requires the use of models largely dependent on vapor pressure data. Since tests with hazardous chemicals may not be possible, reliable calculations are essential. Knowledge of the statistical reliability of vapor pressure data permits engineers to include meaningful safety factors in their designs and analyses.

Due to the high cost of experimental measurements, the purpose of this report is to provide a computation method that yields interpolated and extrapolated values of vapor pressure of the maximum accuracy. Also the objective is to provide 95 % or other confidence intervals and other types of statistics for measured, interpolated and extrapolated values of vapor pressures, boiling points, concentration of saturated vapors, and enthalpies of vaporization. Commercial statistical software packages will perform some of the operations included in this effort, but such packages will not include all the detailed calculations provided here. Furthermore, the detailed, referenced, and complete documentation included here is not provided in most software packages. In addition, this report includes software and plotting compatible with currently available DOS based PCs. Diethyl malonate (DEM) vapor pressure data is used to demonstrate the method.

2. BACKGROUND

2.1 Estimation Methods for the Vapor Pressures of Complex Organic Compounds.

Banerjee, Howard, and Lande,[1] describe a structure-vapor pressure relationship for complex organic compounds that probably is one of the best methods available. Their relationship is based on the following type of parameters: Kamlet-Taft solvatochromic, structural, molecular volume, and UNIFAC. The type of errors in the Banerjee, Howard, and Lande method are given in table 1.

Table 1. Accuracy of the Vapor Pressure Estimation Method of Banerjee, Howard, and Lande.

Compound	% Difference Between Experiment and Calculation
Outliers	
octamethyltetrasiloxane	4,800,000%
ethylene glycol	15,500
hexamethyldisiloxane	11,000
acetic acid	2,137
propionic acid	1,950
diisopropyl ether	1,820
1,1,1-trichloroethane	1,740
hexane	1,300
formic acid	1,200
Typical Errors	500-1,100%

Table 1 illustrates the fact that to obtain data sufficiently accurate for most practical purposes, it is necessary to make at least some measurements at a few temperatures.

2.2 The Antoine Equation.

The Antoine equation[2] is given in equation 1.

$$\log_{10}P = A - B/(t + C) \qquad (1)$$

where

P	= vapor pressure in Torr*
t	= temperature in °C
A, B, C	= constants

For many reasons listed in table 2, the Antoine equation has been selected as the equation of choice for fitting most vapor pressure data.

Table 2. The Advantages and the Disadvantages of the Antoine Equation

Disadvantages

- There is no rigorous theoretical basis for the Antoine equation. (There is no rigorous theoretical basis for any tolerably simple vapor pressure-temperature equation useful for fitting and extrapolating data.)
- It is inadequate for high precision data over the temperature range from the triple point to reduced pressures of 0.75.

Advantages

- It requires only three constants.
- It is quite similar to the Clausius-Clapeyron equation which has an accepted theoretical basis.
- Temperature may be made the dependent variable by a rudimentary inversion.
- Extrapolations and interpolations with the Antoine equation are strikingly more trustworthy than most other equations.
- It may be effortlessly transformed to a linear equation.
- Is the most widely employed equation for fitting vapor pressure measurements.

* Appendix A provides a glossary of terms used in this report.

If X_i and Y_i are defined as follows in equations 2 and 3, the Antoine equation can be transformed into a linear equation (equation 4).

$$X_i = -1/(t_i + C) \quad (2)$$

$$Y_i = \log_{10} P_i = \log_e P_i / \log_e 10 \quad (3)$$

$$Y_i = a_0 + a_1 X_i \quad (4)$$

a_0 and a_1 are constants.

The author and Leo Latour, CRDEC, developed a technique to determine the constants of the linear form of the Antoine equation with a procedure of search by golden section. The method was programmed in FORTRAN to run on a interactive computer with a Typagraph plotter. Since the method was developed in 1971, the program was adapted to several different computer systems at CRDEC. The longest lasting arrangement was with a Unisys 1100/Calcomp plotter system which is scheduled to be removed from service in September 1992. The most recent effort to improve and adapt the program to new computers was performed by Kenneth Collins of CRDEC in 1989. He developed a personal computer version of the program in BASIC and he modified it to be menu driven. No statistics were added by Collins.

The above described software systems have numerous deficiencies that are listed in Table 3.

Table 3. Deficiencies of Currently Available Software

- The number of digits of accuracy required to perform the computation is not calculated. The number of digits required appears to vary from data set to data set. As a result, computer round off error may have a significant effect on the results in some cases.

- In the least squares minimization procedure, more than one minimum may exist that goes undetected.

- Very little statistics is provided. No calculations of 95 % or other confidence limits of boiling points, vapor pressures, volatilities, or enthalpies of vaporization are given. Some of these limits change drastically with temperature and are essential in utilizing the data for practical applications.

- Methodology and references are not kept with each data point. Keeping methodology and references with each data point aids in the analysis of the data.

- No standard deviations of the Antoine constants are provided.

- No correlation coefficient is provided.

- Data editing is difficult.

- Plotting does not include 95 % or other confidence limit envelops.

- The computer that it is written for, the UNISYS 1100, is being removed from service.

2.3 Least Squares Fits.

The statistical treatment used in this report follows references 3 and 4. A linear equation, equation 4, to predict points randomly distributed about a line, is given as follows:

$$Y_i = a_0 + a_1 X_i \tag{5}$$

Summing over all N observed points, yields equation 6.

$$\sum_{i=1,N} Y_i = N a_0 + a_1 \sum_{i=1,N} X_i \tag{6}$$

Dividing equation 6 by N produces equation 7.

$$1/N \sum_{i=1,N} Y_i = a_0 + a_1/N \sum_{i=1,N} X_i \tag{7}$$

To simplify the following analysis, one may let the sums equal S_1, S_2, S_3, S_4, and S_5 as ensues:

$$S_1 = \sum_{i=1,N} X_i \tag{8}$$

$$S_2 = \sum_{i=1,N} X_i^2 \tag{9}$$

$$S_3 = \sum_{i=1,N} X_i Y_i \tag{10}$$

$$S_4 = \sum_{i=1,N} Y_i \tag{11}$$

$$S_5 = \sum_{i=1,N} Y_i^2 \tag{12}$$

The means of X_i and Y_i values are found as follows in equations 13 and 14.

$$\text{Mean of } X_i = \bar{X}_i = 1/N \sum_{i=1,N} X_i = S_1/N \qquad (13)$$

$$\text{Mean of } Y_i = \bar{Y}_i = 1/N \sum_{i=1,N} Y_i = S_4/N \qquad (14)$$

Substituting the mean values from equations 13 and 14 into equation 7 leads to equations 15 and 16.

$$\bar{Y}_i = a_0 + a_1 \bar{X}_i \qquad (15)$$

$$S_4 = N a_0 + a_1 S_1 \qquad (16)$$

The sum, S, of the squared deviations of the calculated Y_i values subtracted from measured values squared is given by equation 17.

$$S = \sum_{i=1,N} (Y_i - a_0 - a_1 X_i)^2 \qquad (17)$$

Squaring the term in parenthesis in equation 17, substituting values from equations 8 to 12, and combining terms yields equations 18 and 19.

$$S = S_5 + N a_0^2 - 2a_0 S_4 - 2a_1 S_3 + 2a_0 a_1 S_1 + a_1^2 S_2 \qquad (18)$$

$$a_1 = (N S_3 - S_1 S_4)/(N S_2 - S_1^2) \qquad (19)$$

Equation 16 rearranges to equation 20.

$$a_0 = (S_4 - a_1 S_1)/N \qquad (20)$$

Equations 18, 19, and 20 permit the easy calculation of S, a_1, and a_0, respectively.

The computer program as developed by the author and Latour varied C and recalculated S until a minimum S was located. Since S represents the difference between calculated and measured values, the C that gave the minimum S was the chosen C. Once C was chosen, a_1 and a_0 were calculated with equations 19 and 20

respectively. The differences in logarithms of vapor pressures as opposed to vapor pressures were minimized to get the fit. Otherwise, the lower values of vapor pressure are ignored by the fitting procedures.

2.4 Statistics of Data Fitted to a Linear Equation.

Natrella[3] defines a number of statistical quantities as follows:

$$\text{Variance} = V_a = S/(N-2) \tag{21}$$

$$\text{Standard deviation of Y over all X's} = \sigma_{Y_i} = V_a^{1/2} \tag{22}$$

D is defined by equation 23.

$$D = N S_2 - S_1^2 \tag{23}$$

$$\text{Standard deviation of slope} = (V_a N/D)^{1/2} \tag{24}$$

$$\text{Standard deviation of intercept} = [V_a (1.0 + S_1^2/D)/N]^{1/2} \tag{25}$$

Correlation coefficient is the square root of the fraction of the squared variation that is explained by the fit to the data.

$$\text{Correlation coefficient} = (1-S/S_9)^{1/2} \tag{26}$$

where

$$S_9 = \sum_{i=1,N} (Y_i - \bar{Y})^2 \tag{27}$$

The variation of the standard deviation of Y_i with X_i and the F-distribution are discussed in reference 4 and Appendix B, respectively. The F-distribution is used to calculate the limits of error at the 95 % or some other confidence level.

2.5 Enthalpy of Vaporization.

The relation of the enthalpy of vaporization (or evaporation) to other variables is usually expressed as the Clapeyron-Clausius equation[5] (equation 28).

$$\frac{dP}{dT} = \frac{\Delta H_v}{T\Delta V_t} \qquad (28)$$

where

T = temperature in Kelvin

ΔH_v = enthalpy of vaporization

ΔV_t = increase in liquid volume on evaporation at temperature t

If the Antoine equation, equation 1, is differentiated with respect to T and substituted into equation 28, the following equation results:

$$\frac{dP}{dT} = \frac{PB \log_e 10}{(C+t)^2} = \frac{\Delta H_v}{T\Delta V_t} \qquad (29)$$

where

$$\Delta V_t = V(\text{vapor}) - V(\text{liquid})$$

In order to compare the two terms, V(vapor) and V(liquid), the "ideal gas law" is introduced.[5] The "ideal gas law" that follows is applicable to vapors at low pressures.

$$PV = nRT$$

where

R = ideal gas law constant
n = number of moles of vapor
V = volume of vapor

In order to establish the relative importance of the two terms, V(vapor) and V(liquid), they are calculated below for DEM at 25 °C.

V(vapor) = RT/P
V(vapor) = 82.05x10^{-6} atm m^3/mol x 298.15 K x 760 Torr/0.2231 Torr
= 83.335 m^3/mol

V(liquid) = molar volume = 160.17 g/mol/(1.0550 g/cc x10^6 cc/m^3)
= 0.0001518 m^3/mol

Since the V(liquid) is over 5 orders of magnitude smaller than V(vapor), V(liquid) can be safely ignored in computing ΔH_v. On substituting V(vapor) for ΔV_t in equation 29 and rearranging terms, equation 30 follows:

$$\Delta H_v = \frac{\log_e 10\ RBT^2}{(C+t)^2} \qquad (30)$$

Equation 30 makes it possible to calculate enthalpies of vaporization from the temperature and the Antoine constants.

2.6 Concentration of Saturated Vapor.

Since the early 20-th century, the term "volatility" has been defined as follows by the military of the world (See Appendix C).

$$\text{Volatility} = PM/RT \qquad (31)$$

Volatility as thus defined is the *concentration of saturated vapor* as calculated from the following variables:

P = saturation vapor pressure
T = absolute temperature in Kelvin
M = compound molecular weight

It is based on the ideal gas law that is fairly accurate at vapor pressures below one atmosphere in pressure. The units of grams or milligrams per cubic meter have been nearly always used. Since many definitions of volatility appear in the literature, the data should be used with caution. Other definitions of volatility that have been used are given in Appendix C.

3. ANALYSIS

3.1 Errors of Vapor Pressure Calculations.

Since the error is extracted from a fit to various types of data, it is assumed in this analysis that all the error is in the vapor pressure values. The experimental temperature control errors are usually so small relative to other errors that they are not reported. The equation for the propagation of errors in terms of variance of vapor pressures, $\Phi_{P_i}^2$, is equation 32.

$$\Phi_{P_i}^2 = \left| dP_i/dY_i \right|^2 \Phi_{Y_i}^2 \tag{32}$$

$\Phi_{P_i}^2$ is a function of X_i, and $\Phi_{Y_i}^2$ is a standard deviation of Y_i that is a function of X_i. Y_i was defined in equation 3.

$$Y_i = \log_{10} P_i \tag{3}$$

Equation 33 is equation 3 rearranged.

$$P_i = 10^{Y_i} \tag{33}$$

Taking the derivative of equation 33 with respect to Y_i yields equation 34.

$$dP_i/dY_i = 10^{Y_i} \log_e 10 = P_i \log_e 10 \tag{34}$$

When equation 34 is substituted into equation 32, equation 35 results.

$$\Phi_{P_i}^2 = (P_i \log_e 10)^2 \Phi_{Y_i}^2 \tag{35}$$

Equation 36 is used to vary the standard deviation with X_1.[4]

$$\Phi_{Y_1}^2 = \sigma_{Y_1}^2 \left[1/N + \frac{(X_1 - S_1/N)^2}{(S_2 - S_1^2/N)} \right] \quad (36)$$

σ_{Y_1} is calculated from equation 22. The error in vapor pressure is given by equation 37.

$$\text{Error in vapor pressure at a given temperature} = \pm (3F)^{1/2} \Phi_{P_1} \quad (37)$$

The value, F, is the percentile value of the F-distribution for the selected confidence level. Appendix B explains how F is calculated at any confidence level.

3.2 Errors of Boiling Point Calculations.

Equation 1, the Antoine equation,

$$\log_{10} P_1 = A - B/(t + C) \quad (1)$$

may be rearranged to provide the boiling point, t_b, as in equation 38.

$$t_b = B/(A - \log_{10} P_1) - C \quad (38)$$

The variance of the boiling point, $\sigma_{t_b}^2$, is calculated with equation 39.

$$\sigma_{t_b}2 = |\delta t_b/\delta P_l|^2 \Phi_{P_l}^2 \quad (39)$$

Taking the derivative of equation 38 with respect to P_l yields equation 40.

$$\delta t_b/\delta P_l = B(A-\log_{10}P_l)^{-2} (P_l \log_e 10)^{-1} \quad (40)$$

On substituting equation 40 into equation 39 and taking the square root yields a standard deviation for the boiling point, σ_{t_b}.

$$\sigma_{t_b} = B(A-\log_{10}P_l)^{-2} (P_l \log_e 10)^{-1} \Phi_{P_l} \quad (41)$$

On substituting equation 35 into equation 41, equation 42 results when P is set at 760 Torr, the vapor pressure at the boiling point under standard conditions.

$$\sigma_{t_b} = B\,(A - \log_{10}760)^{-2}\ \sigma_{Y(760)} \quad (42)$$

$\sigma_{Y(760)}$ is the standard deviation of Y at 760 Torr.

The error in the boiling point is given by equation 43.

$$\text{Error in boiling point} = \pm\,(3F)^{1/2}\,\sigma_{t_b} \quad (43)$$

F is the percentile values of the F-distribution for the the selected confidence level. Appendix B explains how F is calculated at any confidence level.

3.3 Errors in Enthalpy of Vaporization Calculations.

The enthalpy of vaporization may be computed by starting with equation 30.

$$\Delta H_v = RB \log_e 10 \left[(t_1+273.15)/(t_1+C)\right]^2 \qquad (30)$$

The variance of the enthalpy of vaporization is calculated with the following propagation of errors equation:

$$\Phi^2_{\Delta H_v} = \left|\frac{\delta \Delta H_v}{\delta t_1}\right|^2 \left|\frac{\delta t_1}{\delta P_1}\right|^2 \Phi^2_{P_1} + \left|\frac{\delta \Delta H_v}{\delta B}\right|^2 \sigma^2_B + \left|\frac{\delta \Delta H_v}{\delta C}\right|^2 \sigma^2_C \qquad (44)$$

Taking the partial derivative of ΔH_v in equation 30 with respect to t_1 yields equation 45.

$$\left(\frac{\delta \Delta H_v}{\delta t_1}\right)_{B,C} = -2RB \log_e 10 \frac{(t_1+273.15)(C-273.15)}{(t_1+C)^3} \qquad (45)$$

Taking the partial derivative of ΔH_v in equation 30 with respect to B yields equation 46.

$$\left(\frac{\delta \Delta H_v}{\delta B}\right)_{t_1,C} = -R \log_e 10 \left[\frac{t_1+273.15}{t_1+C}\right]^2 \qquad (46)$$

Taking the partial derivative of ΔH_v in equation 30 with respect to C yields equation 47.

$$\left(\frac{\delta \Delta H_v}{\delta C}\right)_{t_1,B} = -2RB \log_e 10 \frac{(t_1+273.15)^2}{(t_1+C)^3} \qquad (47)$$

Taking the partial derivative of t_i in equation 30 with respect to P_i yields equation 48:

$$\left(\frac{\delta t_i}{\delta P_i}\right)_{A,B} = -B(A-\log_{10}P_i)^{-2}(P_i \log_e 10)^{-1} \tag{48}$$

Substituting equations 45-48 into equation 44 yields equation 49.

$$\Phi^2_{\Delta H_v} = \left|2RB^2 \frac{T(C-273.15)}{(t+C)^3(A-\log_{10}P_i)^2 P_i}\right|^2 \Phi^2_{P_i} + \left|R \log_e 10 \frac{T^2}{(t+C)^2}\right|^2 \sigma^2_B + \left|-2RB \log_e 10 \frac{T^2}{(t+C)^3}\right|^2 \sigma^2_C \tag{49}$$

The error in the enthalpy of vaporization at a given temperature is furnished by equation 50.

$$\text{Error in the enthalpy of vaporization at a given temperature} = \pm(3F)^{1/2}\,\Phi_{\Delta H_v} \tag{50}$$

3.4 General Computation Methodology.

The computation is performed differently from previous methods. First a series of values of C are used to calculate a series of S values. Then the S values are searched for minimums and maximums to see if there is more than one minimum. Then the C values are fine tuned to give the C that yields the minimum S. The C that yields the minimum S is then used to calculate the other Antoine constants and the statistics. No effort is made to use an optimized search strategy to conserve computer time since the running time is less than 2 minutes on a Swan Technologies 386/33.

3.5 The Computer Program.

The program used is named "ANT592.BAS" and is written in MS-DOS GW-BASIC for IBM compatible personal computers. The methods of indexing organic compounds and abbreviating references used in the program are given in Appendices D and E respectively. Concentrations of saturated vapor or volatilities (Appendix C) are calculated as a function of temperature. Definitions of the terms used in the program are given in appendix F. The program is listed in Appendix G. When vapor pressure points are entered, an experimental method by which they were obtained and a reference is entered at the same time. The numbers used to represent each method are given in table 4. The data is entered into a BASIC file to preserve the editing capabilities of either GW-BASIC, QBASIC, or any editor that can create a DOS file. The data input format is given in Appendix H.

"ANT592.BAS" produces a "command file" ("ANTPLT.PLT") which includes the data for plotting plus detailed plotting directions. "ANT592.BAS" gives the user a number of options in creating the "command file." After "ANT592.BAS" is run, the user must terminate GW-BASIC with a "SYSTEM" command and switch to "ProPLOT" software. In "ProPLOT" the user may view the plots on the screen before plotting, edit the plots, and send them to a laser printer. "ProPLOT" is a 2-D scientific plotting software package sold by Cogent Software that creates PostScript printer output.

Table 4. The Numbers Used to Represent Each Experimental Method.

Number	Method
1	Isoteniscope
2	Boiling Point
3	Effusion
4	Dynamic Gas Saturation
5	Manometer
6	Tensimeter
7	Gas Chromatography
8	DTA
9	Ebulliometry
10	Calculated
11	Method Not Given
12	Droplet Evaporation

4. RESULTS

A sample calculation for DEM is provided in Appendix I.

Brozena and Fielder's[6] data for DEM was chosen to demonstrate the methodology. As is apparent from Appendix I, the fit is good and there are more statistically significant digits, three, available than is normally expected from vapor pressure data. At least three digits for the enthalpy of vaporization are significant and four should be reported. The error estimation techniques used are worst case methods; they are so inclusive that errors are probably over-estimated.

Figure 1 shows that a plot of logarithm of vapor pressure versus -1/(t+C) which gives a very linear plot of the data. The data fits the Antoine equation fit so well that the error bars are expanded 20 times the actual error limits to permit their being easily observable. Clearly the DEM data is excellent. Figures 2-6 provide simple vapor pressure versus temperature plots with error bars.

The program "ANT592.BAS" takes about 20 minutes running time more or less on a number of early model IBM compatible PCs, but on a Swan 386/33 it runs in minute or so. The program has estimated that ten decimal digits accuracy is required for the DEM data set.

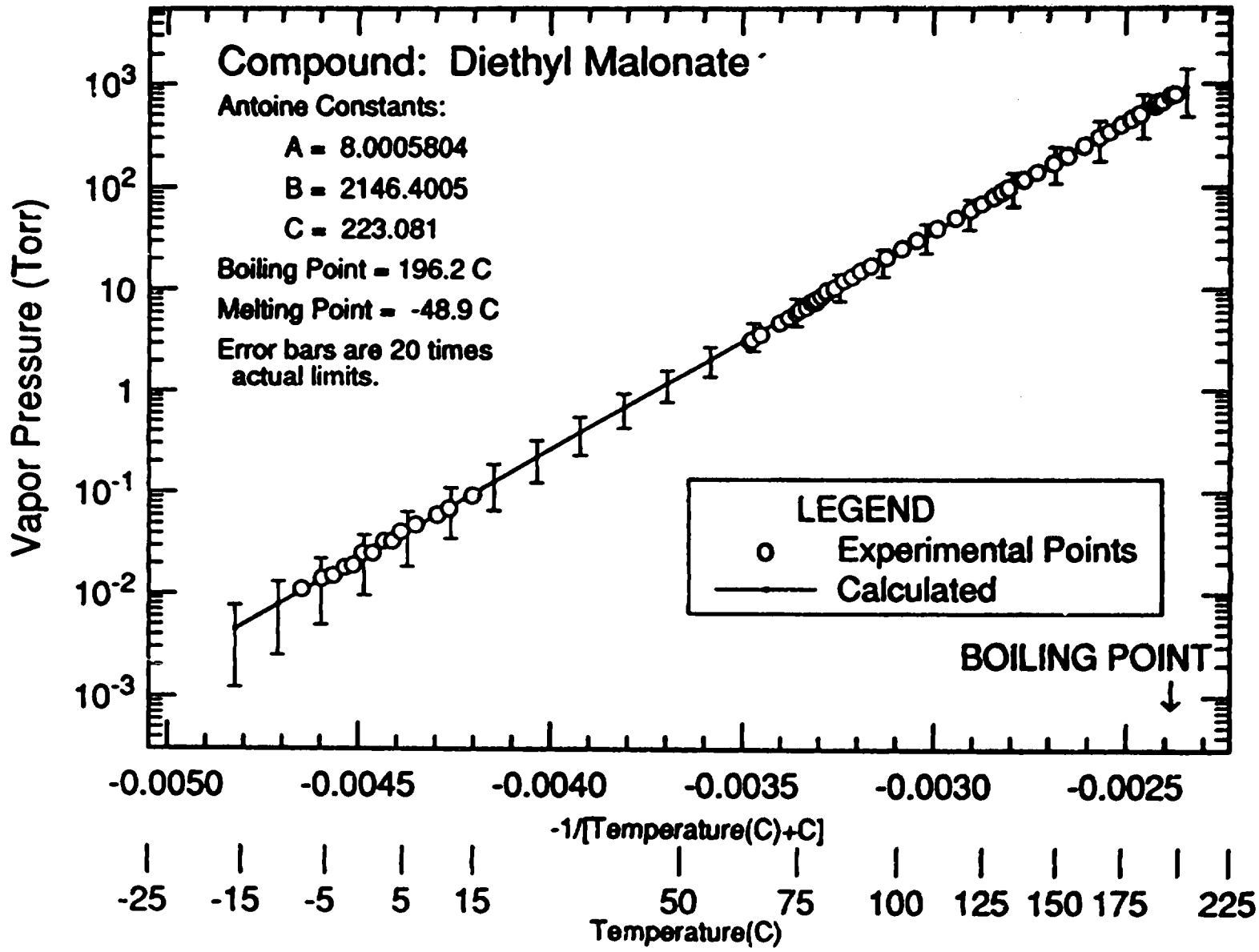

Figure 1. Comprehensive Plot of Logarithm of Vapor Pressure Versus -1/(t+C)

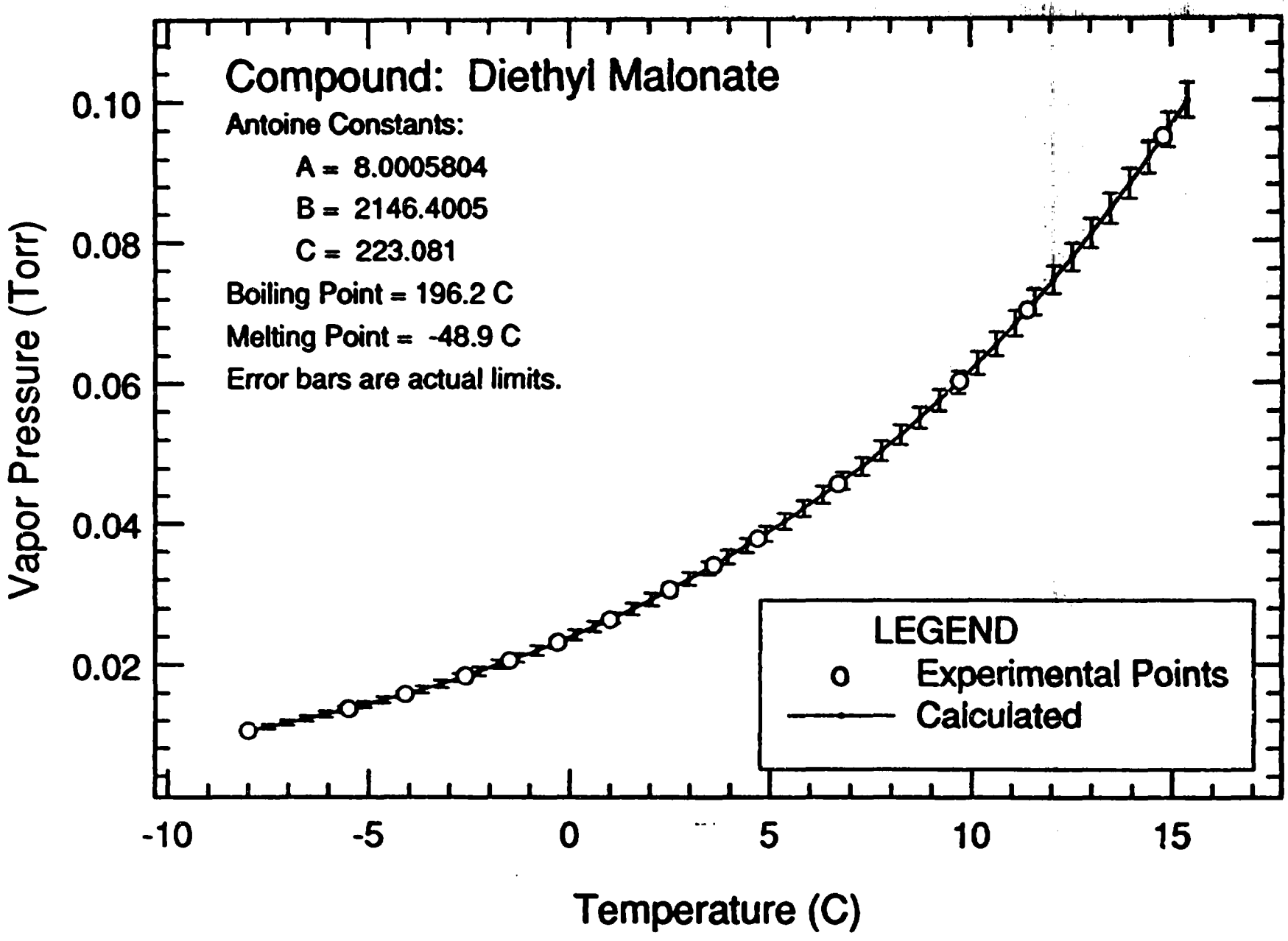

Figure 2. Vapor Pressure Versus Temperature Plot from 0.01 to 0.1 Torr

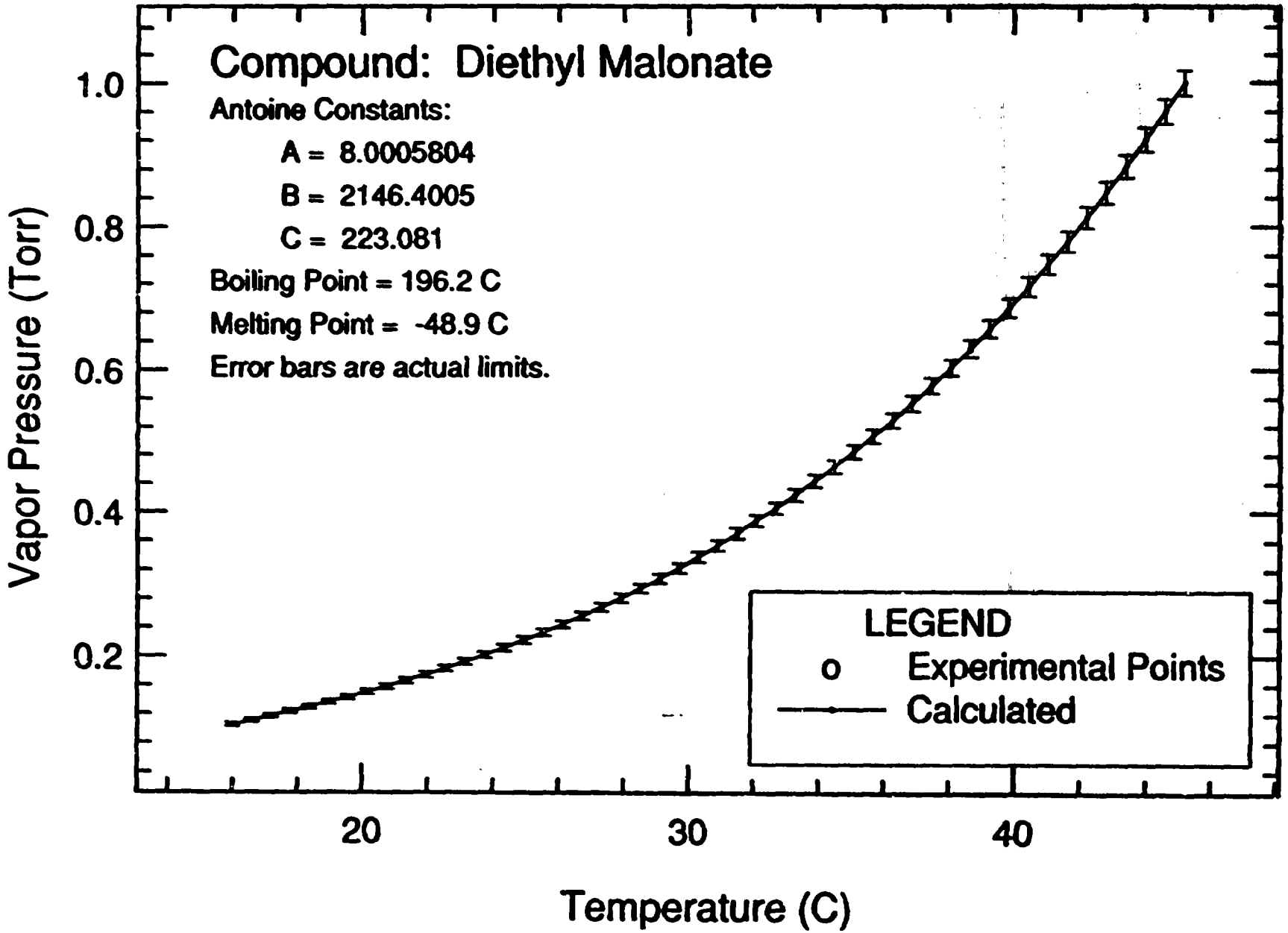

Figure 3. Vapor Pressure Versus Temperature Plot from 0.1 to 1.0 Torr

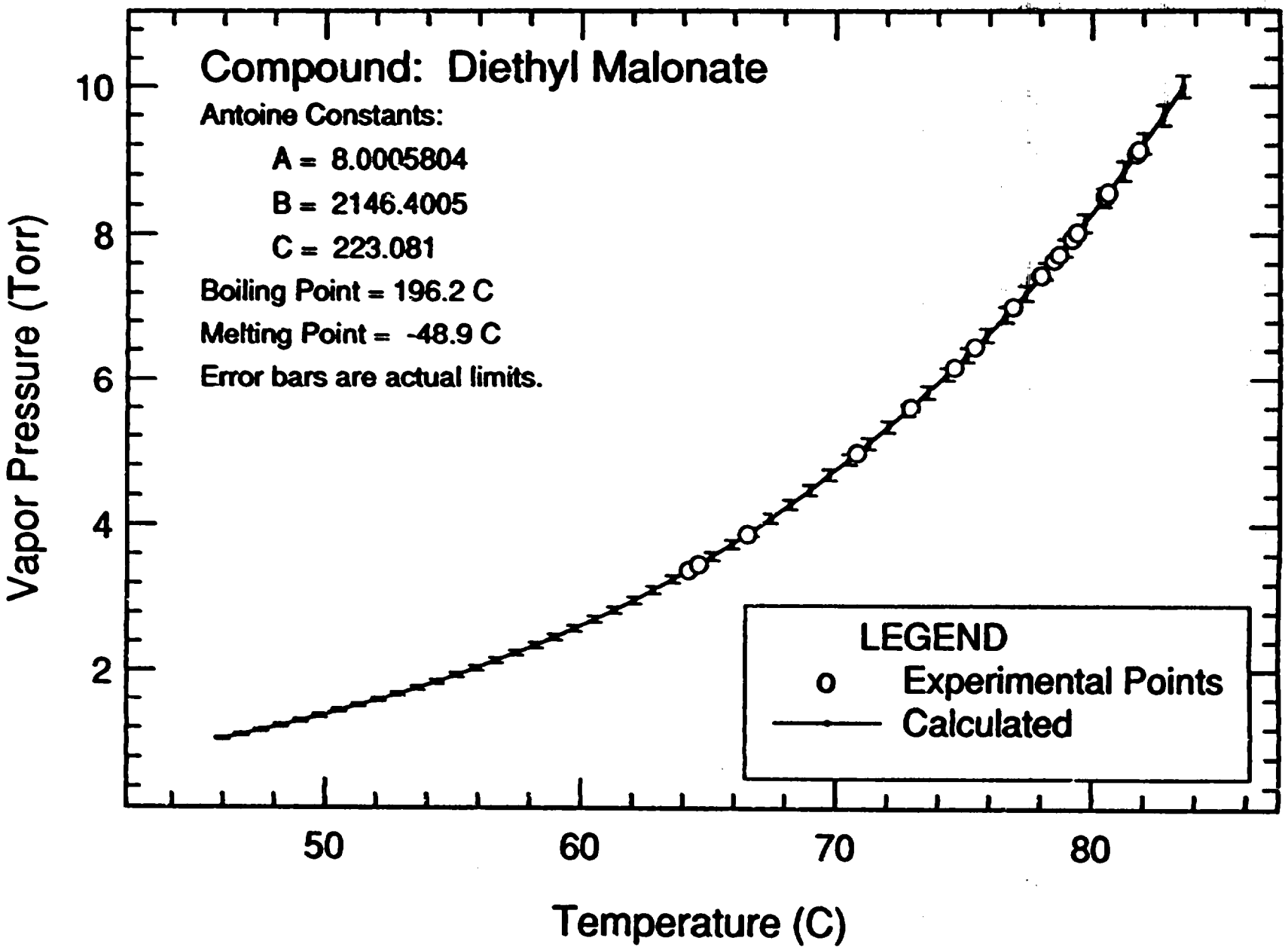

Figure 4. Vapor Pressure Versus Temperature Plot from 1.0 to 10. Torr

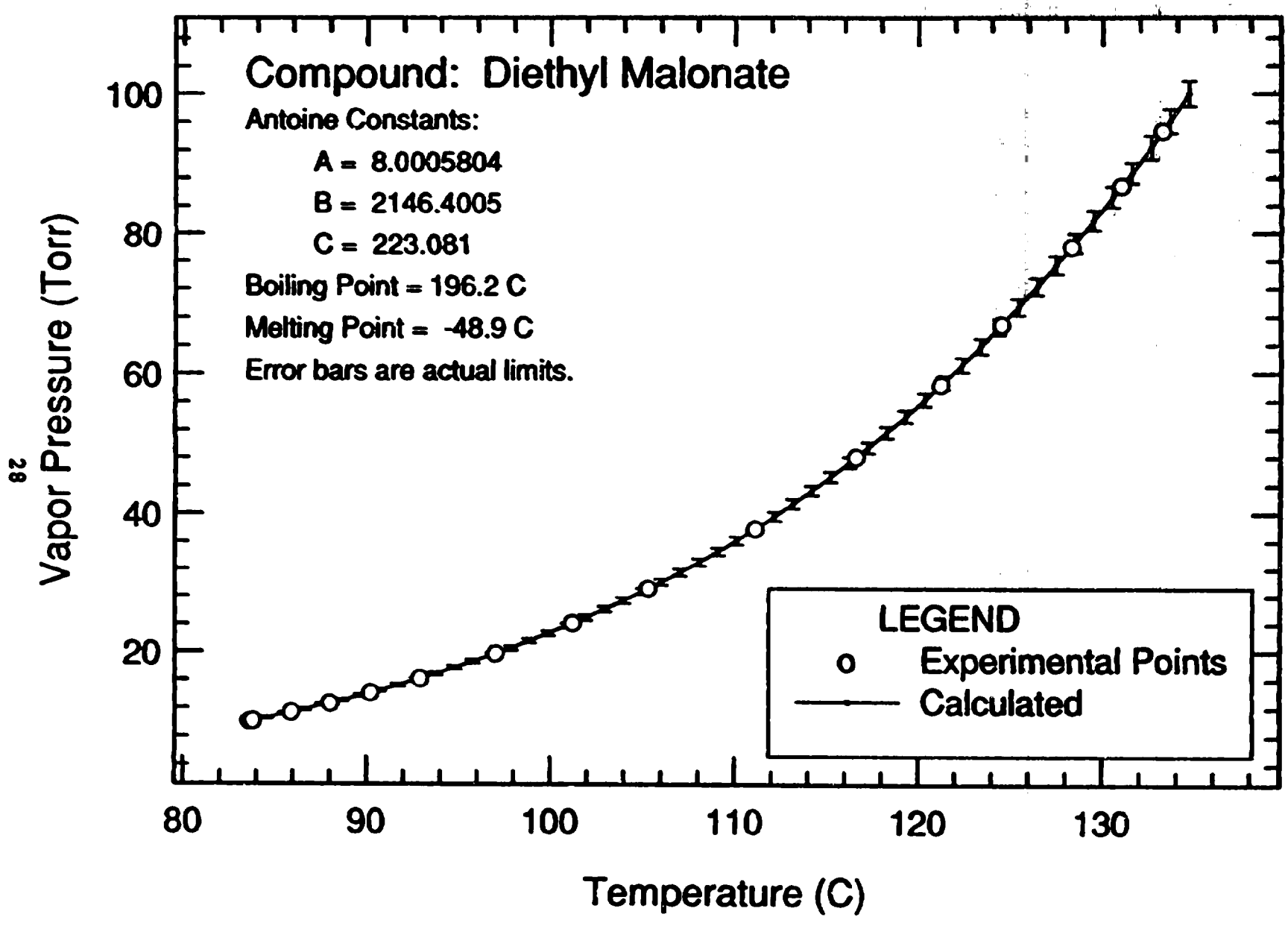

Figure 5. Vapor Pressure Versus Temperature Plot from 10.0 to 100. Torr

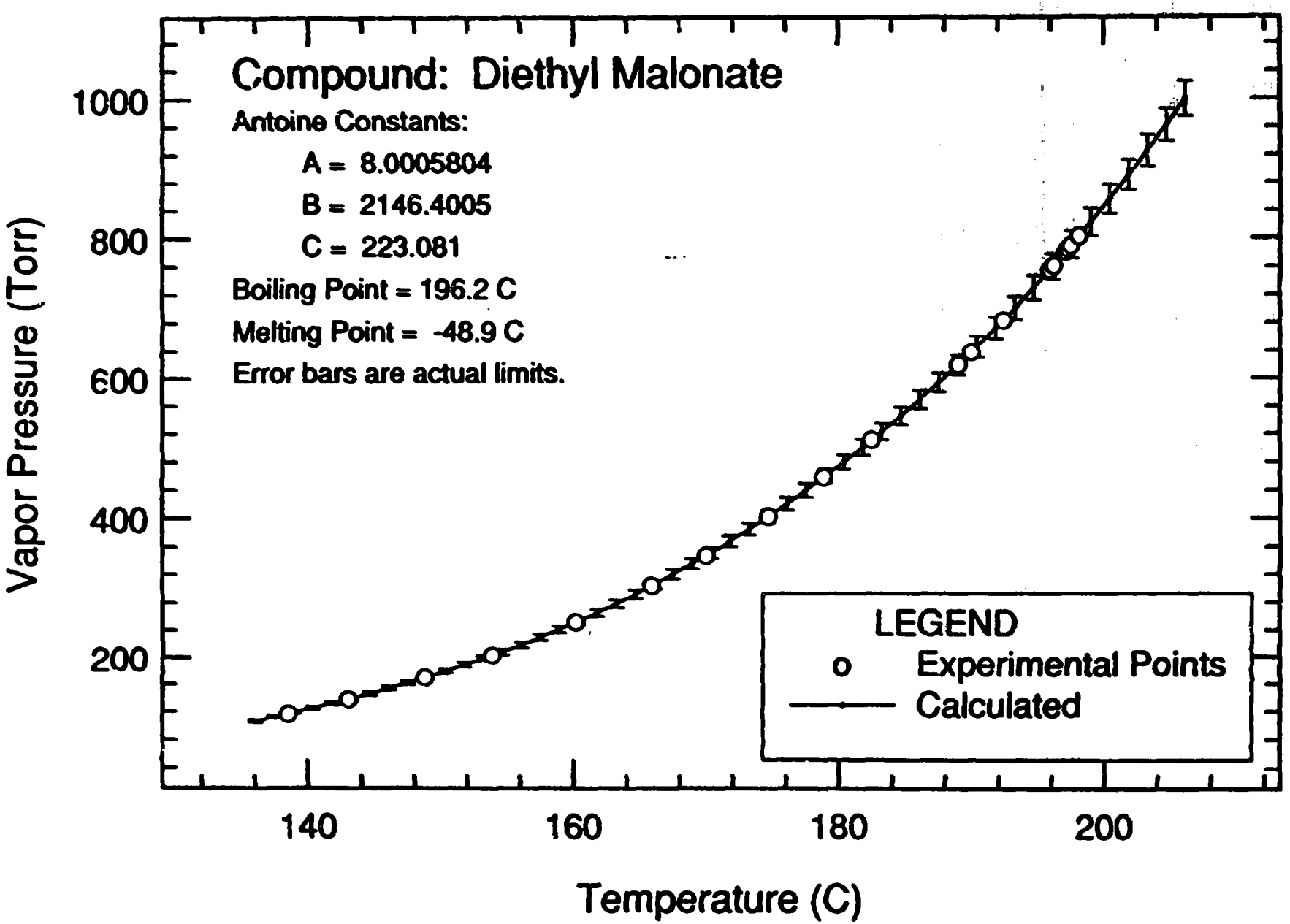

Figure 6. Vapor Pressure Versus Temperature Plot from 100. to 1000. Torr

5. DISCUSSIONS

In MS-DOS GW-BASIC for IBM compatible personal computers, single precision goes from 10^{-38} to 10^{+38} with 6 decimal digits and double precision covers the same range with 16 decimal digits. The program calculates the number of digits required to avoid significant round off errors. Since twelve digits were required for the DEM data given in this report and as many as 14 digits with other sets of data were required, double precision is definitely necessary for an Antoine fit.

Statistical error analysis is often a much larger task than making measurements and analyzing the data without statistics.

In addition to being used to fit vapor pressure data, the Antoine may be used to fit densities, fugacities of liquids, viscosities, relative vapor pressures, and other types of data. The only time that the program was found to give more than one minimum was when it was run in the single precision mode.

The analysis performed in this report shows that Brozena and Fielder's[6] data for DEM is one of the best series of vapor pressure data found anywhere in the scientific literature.

6. CONCLUSIONS

- The program "ANT592.BAS" performs all the calculations of previous programs satisfactorily, plus it provides detailed statistical analysis and error envelopes for any confidence level for vapor pressures, enthalpies of vaporization, concentrations of saturated vapor, and boiling points.

- More statistically significant decimal digits are available for vapor pressure data, three, than has been previously believed. In the future four digits should be published.

- Five decimal digits for the enthalpy of vaporization values are significant and should be reported.

- Double precision computations (10-16 decimal digits) are required for maintaining the full significance of carefully measured vapor pressure data.

- The ANT592.BAS"/"ProPLOT" system produces greatly improved plots with error limits.

LITERATURE CITED

1. Banerjee, S., Howard, P.H., and Lando, S.S., "General Structure-Vapor Pressure Relationships for Organics," Chemosphere, Vol. 21, Nos. 10-11, 1173 (1990).

2. Thomson, G.W., "The Antoine Equation for Vapor Pressure Data," Chemical Reviews, Vol. 38, 1 (1946).

3. Ostle, B., and Mensing, R.W., Statistics in Research, Third Edition, The Iowa State University Press, Ames, Iowa, 1975.

4. Natrella, M.G., Experimental Statistics, National Bureau of Standards (NBS) Handbook 91, NBS, U.S. Department of Commerce, Gaithersburg, MD, October 1966.

5. Moore, W.J., Physical Chemistry, Fourth Edition, Prentice-Hall, Inc., Englewood Cliffs, NJ, p 211, 1972.

6. Brozena, A. and Fielder, D., Vapor Pressure of Diethyl Malonate, CRDEC-TR-120, November 1989, UNCLASSIFIED Report

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APPENDIX A

GLOSSARY OF TERMS

A	= constant for the Antoine equation, equation 1
a_0	= intercept in equation 4
a_0	= slope in equation 4
B	= constant for the Antoine equation, equation 1
C	= constant for the Antoine equation, equation 1
D	= value defined by equation 23
F	= percentile value of the F-distribution for the selected confidence level
ΔH_v	= enthalpy of vaporization
M	= molecular weight of vapor
N	= number of observed points
n	= number of moles of vapor
P	= vapor pressure in Torr
R	= ideal gas law constant
S	= sum of the deviations of the Y values squared, defined by equation 17
S_1	= sum of X_i s, defined by equation 8
S_2	= sum of X_i^2 s, defined by equation 9
S_3	= sum of X_iY_i s, defined by equation 10
S_4	= sum of Y_i s, defined by equation 11
S_5	= sum of Y_i^2 s, defined by equation 12
S_9	= value defined by equation 27

t = temperature, °C

T = temperature in Kelvin

t_b = boiling point, °C

V = volume of vapor

V_a = variance of Y_i s

ΔV_t = Change in volume of a given amount of fluid on evaporation at a given temperature and pressure

X_i = $-1/(t_i + C)$

$\bar{X}_i$ = mean of X_i s

Y_i = $\log_{10} P_i$

$\bar{Y}_i$ = mean of Y_i s

σ_B = standard deviation of B

σ_C = standard deviation of C

$\sigma_{\Delta H_v}$ = standard deviation of enthalpy of vaporization

σ_{t_b} = standard deviation of boiling point

σ_{Y_i} = standard deviation of Y_i s

$\phi_{\Delta H_v}$ = standard deviation of enthalpy of vaporization that is a function of t

ϕ_{P_i} = standard deviation of vapor pressures that is a function of t

ϕ_{Y_i} = standard deviation of Y_i that is a function of the size of X_i or t_i.

APPENDIX A

APPENDIX B

CALCULATION OF F FROM F-DISTRIBUTION

Equation 1 provides the equation that is integrated to the required level of confidence to obtain the standard statistical value, F.[1]

$$f(F) = \int_0^F \left[\frac{\Gamma\left(\frac{u+v}{2}\right) u^{\frac{u}{2}} v^{\frac{v}{2}} F^{\frac{u}{2}-1} (v+uF)^{-\frac{u+v}{2}}}{\Gamma\left(\frac{u}{2}\right)\Gamma\left(\frac{v}{2}\right)} \right] dF \qquad (1)$$

where:

$f(F)$	= F-distribution
Γ	= gamma functions
u	= degrees of freedom in the numerator of F
v	= degrees of freedom in the denominator of F

The gamma function, Γ, was calculated with the following equation:[2]

$$\log_e \Gamma(x) = \left(x - \frac{1}{2}\right)\log_e x - x + \frac{1}{2}\log_e(2\pi) + \frac{1}{12x} - \frac{1}{360x^3} + \frac{1}{1260x^5} - \frac{1}{1680x^7} \qquad (2)$$

where x is the argument of the gamma function.

For the calculations for errors in this report v is taken as the number of points minus three and u is taken as three.

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1. Beyer W.H., Handbook of Tables for Probability and Statistics, The Chemical Rubber Company, Cleveland, Ohio, p304, 1968.
2. Abramowitz, M. and Stegun, I.A., Handbook of Mathematical Functions, Applied Mathematics Series 55, National Bureau of Standards, Washington, D.C., p257, 1970.

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APPENDIX C

DEFINITION OF VOLATILITY OR CONCENTRATION OF SATURATED VAPOR

Parker[1] claims volatility is a thermodynamic quantity with the following qualitative definition: "The quality of having a low boiling point or subliming temperature at ordinary pressure or equivalently, of having a high vapor pressure at ordinary temperatures."

According to Bridgeman[2] of the National Bureau of Standards the "volatility of gasoline is the temperature at which a given air-vapor mixture is formed under equilibrium conditions at a pressure of one atmosphere, when a given percentage is evaporated."

The Kirk-Othmer Encyclopedia of Chemical Technology[3] deals with volatility as follows. "The volatility of kerosine fuel is measured not by its vapor pressure but by its temperature at the point where its vapors prove to be flammable, ie, the flash point or lean flammability temperature."

Some reports seem to use the Reid vapor pressure as a measure of volatility. It is defined by the U.S. Coast Guard[4] as the equilibrium vapor pressure exerted by vapor over the liquid at 100 °F., expressed as pounds per square inch absolute, as defined by the 46 Code of Federal Regulations 30.10-59.

The United Nations[5] defined volatility as the concentration of saturated vapor at 20 °C in units of mg/m^3. This the standard definition used by the military of most nations, but the U.S. Coast Guard[4] refers to this quantity as the saturated vapor density.

Volatility has been historically defined as follows by the U.S. Department of Defense:

$$\text{Volatility} = PM/RT$$

This is the concentration of vapor as calculated from the vapor pressure, P, and the absolute temperature, T. It is based on the ideal gas law that is fairly accurate at vapor pressures below one atmosphere in pressure. The units of grams or milligrams per cubic meter have always been used.

Since the term volatility has multitude of definitions in the literature, it is recommended that "volatility" not be used by the U.S. Army in the future and the term "concentration of saturated vapor" at a given temperature be used instead. The units should remain grams or milligrams per cubic meter.

LITERATURE CITED

1. Parker, S.P., McGraw-Hill Dictionary of Scientific and Technical Terms, 4th Edition, McGraw-Hill Book Company, New York, 1989.

2. Considine, D.M., and Considine, G.D., Encyclopedia of Chemistry, 4th Edition, Van Nostrand Reinhold Company Inc., p701, 1984.

3. Kirk, R.E., et al, Kirk-Othmer Encyclopedia of Chemical Technology, Vol. 3, John Wiley & Sons Inc., New York, p343, 1978.

4. CHRIS Hazardous Chemical Data, U.S. Department of Transportation, U.S. Coast Guard, Commandant Instruction, M.16465.12A, November 1984.

5. Secretary-General, Chemical and Bacteriological (Biological) Weapons and the Effects of Their Possible Use, United Nations, New York, p90, 1969.

APPENDIX C

APPENDIX D

EMPIRICAL FORMULA INDEXING OF ORGANIC COMPOUNDS

Generally the simplest way to index organic compounds is a empirical formula index (better named an elemental formula). This index that is usually used to locate compounds is given as follows:

$$C_nH_mX_oY_pZ_q$$

where

C	= Carbon
n	= Number of carbon atoms in molecule
H	= Hydrogen
m	= Number of hydrogen atoms in molecule
X,Y,Z	= Elements other than carbon and hydrogen (Usually given in alphabetical order)
o,p,q	= Number of elements other than carbon and hydrogen

The elemental formula are listed in alphabetical and numerical order(lower numbers first). Lange's Handbook of Chemistry provides examples.*

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* Dean, J.A., Lange's Handbook of Chemistry, 13th ed., McGraw-Hill Book Co., New York, page 7-54, 1985.

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APPENDIX E

CHEMICAL THERMODYNAMICS DATA CENTER (NIST) REFERENCE CODE

The following method of handling references* has been found to be more useful than simply numbering references:

Code: XXAAA/BBB N

where

XX = Last two digits of year

AAA = First 3 letters of the last name of first author

BBB = First 3 letters of the last name of second author

N = Digit from 2 to 9 used to represent a second or third paper of the first and second author in the same year.

Thus 60ADA/BRO 4 would be used to represent the 4-th paper by Adams and Brown in 1960 referenced in the report. 80SMI would represent the only paper by Smith in 1980 referenced in the report.

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* Domalski, E.S., Evans, W.H., and Hearing, E.D., "Heat Capacities and Entropies of Organic Compounds in the Condensed Phase," J. Phys. Chem. Ref. Data Vol. 13, Suppl. 1 (1984).

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APPENDIX F

DEFINITIONS OF COMPUTER TERMS

A#	= A
ABCMK	= absolute value of C - 273.15
ARG#	= argument of Gamma function
AT$(I)	= atomic symbol
ATOM$(I)	= atomic symbol
AW#(I)	= atomic weight
B#	= B
B9#	= degree of precision required in C
BASETEN#	= natural logarithm of 10 (double precision)
BP	= boiling point, Celsius
BP3	= 90 % plus or minus deviation of boiling point
BTEN	= natural logarithm of 10
C#	= C
C$(I)	= reference for each data point
C2#	= calculated vapor pressure
CA#(I)	= a set of C's selected for locating minimum
CA2#(I)	= a set of C's for fine tuning
CAA#	= the C being tested for locating minimum
CAMIN#	= the minimum C in the set DA#(I)
COMPOUND$	= compound name
CON#	= constant, 0.0019872 $\log_e 10$
CORCO	= correlation coefficient

D# = $n S_2 - S_1^2$

D3 = 95 % or other confidence limit deviation in vapor pressure

DC# = increment in C used fine tune C

DIC# = double precision integer used in fine tuning C

DIST = distance along Celsius axis for plotting

ELFORMULA$ = elemental formula

FCONF# = % confidence level chosen/100

FF# = F

FILES$ = name of file containing experimental data

G#(I) = experimental vapor pressure at I-th temperature, Torr

H# = highest temperature chosen to calculate properties, Celsius

HEAT = enthalpy of vaporization

ICMIN = an integer for minimum C in the CA#(I) set

INTERVAL# = the number of degrees chosen between calculation of properties

KEL = 273.15

KELVIN# = 273.15, double precision

L# = lowest temperature chosen to calculate properties, Celsius

L1# = logarithm of Gamma function

L2# = term in Gamma function

LOGGAMMA = L1#

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M$(I)	= verbal description of the experimental method
M(I)	= code number used to represent experimental method
MW#	= molecular weight
N	= number of experimental points
N2#	= number of experimental points, double precision
N8	= n9-1
N9	= number of C's calculated in search of maximums or minimums
NDIG	= $S/(S_I - S_{I-1})$
NIT	= number of iterations
NMIN	= number of minima found
NOTHING	= dummy variable designed to provide a pause
NP	= controls the number of points per line
NUMBERATOMS	= number of atoms of each type in a molecule
NUMBEREL	= number of elements in compound
PCD#	= % difference between calculated and measured vapor pressures
PRC#	= calculated vapor pressure
R#	= R, ideal gas law constant, 0.082053
RS	= R, ideal gas law constant, 0.0019872
RTC	= 1/(t+C)
S#	= S
S1#	= S_1
S2#	= S_2
S3#	= S_3

APPENDIX F

S4# = S_4

S5# = S_5

S9# = S_9

SD# = standard deviation of Y_is

SIGH = standard deviation of enthalpy of vaporization

SIGHB = contribution of B to the variance of the enthalpy of vaporization

SIGHC = contribution of C to the variance of the enthalpy of vaporization

SIGHP = contribution of P to the variance of the enthalpy of vaporization

ST = F

STDEVA = standard deviation of A

STDEVB = standard deviation of B

T#(I) = experimental temperature, Celsius

T1# = temperature for calculations, Celsius

TK# = temperature in Kelvin

TPC = temperature in Celsius plus Antoine constant C

U# = u

U2# = u/2

U$ = Y or N (yes or no)

UV# = (u+v)/2

V#(I) = array of initial S values

V2#(I) = array of S values for fine tuning

V# = v

APPENDIX F

VAR	= variance of Y_is
VOL	= volatility
W1#	= minimum value of C considered
W2#	= maximum value of C considered
W3#	= lowest C in a CA2#(I) set
X#	= X_i
XMAX	= maximum value of X_i used in plotting
XMIN	= minimum value of X_i used in plotting
XX#	= value used to calculate F
Y#(I)	= Y_i
Y$	= selector taking values of Y(yes) or N(no).
YY#	= Y_i
Z#	= value used to calculate F
ZSD	= $\sigma_{Y_i}^2$
ZX	= $-1/(t + C)$
ZZZ	= $A - \log_{10}760$

APPENDIX F

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APPENDIX G

COMPUTER PROGRAM

```
10 REM Program Name: ANT592.bas          Programmed by: El Penski
20 REM Language:     MS-DOS, BASIC       Computer:      SWAN 386/33
30 REM Directions:   Store data in BASIC program starting with
                       line 4000.  To enter BASIC, type BASICA/d
40 REM               See Appendix H for data input format.
50 REM               Save with "A" option -- SAVE "XXXXX",A --
60 REM               To run LOAD "ANT592"; MERGE "XXXXX"; and
                       type RUN
70 REM               To run with printer type ([Ctrl] [Print
                       Scrn]) and RUN
80 REM               Command file for ProPLOT is stored in
                       "A:\Antplt.plt"
90 REM               After run, type "SYSTEM" to leave BASIC.
100 REM              At the A:> type "C:\Pro\ProPLOT" to plot.
110 REM              Enter command files, translate, view, and
                       plot.
120 REM
```

```
130 PRINT "ADVANCED VAPOR PRESSURE DATA ANALYSIS AND PLOTTING"
140 PRINT : PRINT "  PROGRAM: ANT592.BAS"
150 REM ***** Initialize Terms *****
160 BASETEN# = LOG(10#): B9# = .001#: BTEN = LOG(10): RPT = 12
170 R# = .082053#: CON# = .0019872# * BASETEN#: RS = .0019872:
      FCONF# = .95#
180 S4# = 0#: S5# = 0#: KELVIN# = 273.15#
190 REM ***** Test Double Precision *****
200 TEST1# = 1.0000000000001#: TEST2# = TEST1#: TEST# = TEST1# *
      TEST2# - 1#
210 IF TEST# = 0# GOTO 220 ELSE 230
220 PRINT "Double precision problem "
230 REM ***** Select Type of Output *****
240 PRINT "Run date is "; DATE$
250 PRINT "Is 95% confidence level OK? (Y or N) "; : INPUT U$
260 IF U$ = "y" OR U$ = "Y" GOTO 290 ELSE 270
270 PRINT "What confidence level do you want?  Answer in %."; :
      INPUT FCONF#
280 FCONF# = FCONF# / 100#: PRINT
290 PRINT USING "The ###.# % confidence level was chosen.";
      FCONF# * 100
300 INPUT "Do you intend to plot? (Y or N) "; U$
310 IF U$ = "y" OR U$ = "Y" GOTO 320 ELSE 330
320 OPEN "a:\antplt.plt" FOR OUTPUT AS #1
330 DIM T#(100), G#(100), Y#(100), C$(100), M(100), CA#(200),
      V#(200)
340 DIM AT$(20), ATOM$(20), AW#(20), M$(20), V2#(6), CA2#(6)
```

```
350 REM*****SET UP MOLECULAR WEIGHT CALCULATION
360 FOR I = 1 TO 10: READ AT$(I), AW#(I): NEXT I: MW# = 0
370 DATA  "C",12.011,"H",1.0079,"Br",79.904,"Cl",35.453,"F",
    18.9984
380 DATA "N",14.0067,"O",15.9994,"P",30.9738,"S",32.06,"Si",
    28.086
390 REM*****INPUT METHOD NAMES
400 M$(1) = "Isoteniscope": M$(2) = "Boiling Point": M$(3) =
    "Effusion"
410 M$(5) = "Manometer": M$(4) = "Dynamic Gas Saturation": M$(6)
     = "Tensimeter"
420 M$(7) = "Gas Chromatography": M$(8) = "DTA": M$(9) =
    "Ebulliometry"
430 M$(10) = "Calculated": M$(11) = "Method Not Given"
440 M$(12) = "Droplet Evaporation": PRINT : PRINT
450 PRINT "Element  Atomic Weight"; SPACE$(11); "Number
    Experimental Method"
460 PRINT : FOR I = 1 TO 12: REM Output Atomic Weights and Method
     Keys
470 PRINT USING "\  \     ###.#####"; AT$(I); AW#(I);
480 PRINT USING "                  ##       &"; I; M$(I)
490 NEXT I: PRINT : PRINT
500 READ ELFORMULA$: PRINT "Elemental Formula = "; ELFORMULA$;
    SPACE$(5);
510 READ NUMBEREL, N: FOR I = 1 TO NUMBEREL
520 READ ATOM$(I), NUMBERATOMS#(I): FOR J = 1 TO 10
530 IF ATOM$(I) <> AT$(J) GOTO 560 ELSE 540
540 MW# = MW# + NUMBERATOMS#(I) * AW#(J)
550 GOTO 570
560 NEXT J: PRINT : PRINT "Element not in file", ATOM$(I)
570 PRINT AT$(J); NUMBERATOMS#(I); : N2# = CDBL(N)
580 NEXT I: READ COMPOUND$, MP#:
590 PRINT : PRINT "Calculated Molecular Weight of "; COMPOUND$; "
    = "; MW#
600 GOSUB 820
610 PRINT "          Experimental Data, Methods, and References
     for"
620 PRINT "                "; COMPOUND$
630 N2# = CDBL(N)
640 GOSUB 770
650 PRINT "     Temper-       Vapor"
660 PRINT "      ature       Pressure      Reference
    Method"
670 PRINT "     Celsius        Torr"
680 GOSUB 770
690 REM ***** Read and Print Input *****
700 FOR I = 1 TO N: READ T#(I), G#(I), C$(I), M(I)
710 PRINT USING "      ###.#      ##.###^^^^  "; T#(I); G#(I);
720 PRINT USING "   \           \ "; C$(I);
```

```
730 PRINT USING " \                          \ "; M$(M(I))
740 Y#(I) = LOG(G#(I)) / BASETEN#
750 NEXT I: GOSUB 770: GOSUB 3510: GOTO 850
760 REM ***** SUBROUTINE - LINE MAKER *****
770 PRINT SPACE$(5); : GOTO 790
780 PRINT "_____";
790 PRINT "_____"
800 PRINT : RETURN
810 REM ***** SUBROUTINE - Pause and Start a New Page *****
820 PRINT : INPUT "Hit Enter or Return Key"; NUTIN: PRINT
      CHR$(RPT): RETURN
830 REM Define range of search
840 REM ***********************************
850 W1# = 50#: W2# = 600#: N9 = 55: PRINT CHR$(RPT)
860 PRINT "**********EVALUATE"; N9; "C's FOR MAXIMUMS AND
      MINIMUMS**********"
870 PRINT "This is helpful only with a narrow temp. range or poor
      data."
880 PRINT : GOSUB 890: GOSUB 890: GOSUB 890: PRINT : GOTO 900
890 PRINT "    C       S                ";  : RETURN
900 NP = 0: NMIN = 0
910 FOR IC = 1 TO N9: DIC# = CDBL(IC) - 1#: CA#(IC) = W1# + (W2#
      - W1#) * DIC# / CDBL(N9)
920 CAA# = CA#(IC): GOSUB 3260: V#(IC) = S#
930 PRINT USING "###.# ##.##############  "; CA#(IC); V#(IC); : NP
      = NP + 1
940 IF NP = 3 GOTO 950 ELSE 960
950 PRINT : NP = 0
960 NEXT IC: N8 = N9 - 1
970 REM    ***** FIND LOWEST C IN 30 C's*****
980 FOR IC = 2 TO N8:
990 IF V#(IC) < V#(IC - 1) GOTO 1000 ELSE 1010
1000 IF V#(IC) < V#(IC + 1) GOTO 1030 ELSE 1040
1010 IF V#(IC) < V#(IC + 1) GOTO 1040 ELSE 1020
1020 PRINT "max C="; V#(IC): GOTO 1040
1030 ICMIN = IC: CAMIN# = CA#(ICMIN): NMIN = NMIN + 1
1040 NEXT IC
1050 PRINT : PRINT : PRINT "C for minimum S = "; CAMIN#
1060 PRINT "Minimum S = "; V#(ICMIN)
1070 PRINT "Number of minimums = "; NMIN
1080 IF NMIN <> 1 GOTO 1090 ELSE 1110
1090 INPUT "*** PROBLEM *** Look at minimums! *** Select C >";
      CAMIN#
1100 PRINT "C set as provided by user.": GOTO 1330
1110 PRINT : PRINT "********** FINE TUNING OF C **********"
1120 FOR J = 1 TO 17
```

```
1130 PRINT USING " ###.###"; CAMIN#;
1140 DC# = (W2# - W1#) * 2.1# * ((.5#) ^ (J - 1)) / CDBL(N9)
1150 IF DC# < B9# GOTO 1260 ELSE 1160
1160 W3# = CAMIN# - DC# / 2#
1170 FOR IC = 1 TO 5
1180 DIC# = CDBL(IC) - 1#: CA2#(IC) = W3# + DC# * DIC# / 4#
1190 CAA# = CA2#(IC): GOSUB 3260: V2#(IC) = S#
1200 NEXT IC
1210 FOR IC = 2 TO 5
1220 IF V2#(IC) > V2#(IC - 1) GOTO 1240 ELSE 1230
1230 NEXT IC: IC = 6
1240 ICMIN = IC - 1: CAMIN# = CA2#(ICMIN)
1250 NEXT J
1260 PRINT : PRINT : PRINT "          Review of Fitting
       Process": GOSUB 790
1270 PRINT USING "Final C = ###.#### at an Interval of ##.#####";
       CAMIN#; DC# * 2.1
1280 PRINT USING "Final S = ##.############## after ##-th step";
       V2#(ICMIN); J
1290 PRINT "Number of digits required in calculation";
1300 NDIG = V2#(3) / (V2#(3) - V2#(2))
1310 IF NDIG < 0! THEN NDIG = -NDIG
1320 PRINT USING " is ### "; 2.5 + LOG(NDIG) / LOG(10)
1330 C# = CAMIN#: GOSUB 3370: GOSUB 3210: GOSUB 790
1340 PRINT "                          RESULTS": PRINT
1350 PRINT "Antoine Constants for "; COMPOUND$; ":"
1360 PRINT USING "   A = ##.#######  B = #####.#####  C =
       ####.###"; A#; B#; C#
1370 VAR = S# / (N2# - 2#)
1380 SD# = SQR(VAR): BP = -B# /(2.88081# - A#) - C#: T1# = BP: ZX
       = -1 / (T1# + C#)
1390 ZSD = SQR(VAR * (1/N2# + ((ZX - S1# / N2#) ^ 2) / (S2# - S1#
       ^ 2 / N2#)))
1400 ZZZ = A# - (LOG(760) / LOG(10))
1410 BP3 = SQR(3# * F#) * B# * ZSD / (ZZZ ^ 2): PRINT
1420 PRINT USING "Standard Deviation of A = ##.###### "; STDEVA;
1430 PRINT USING " and of B = #####.###"; STDEVB
1440 PRINT USING "F = ###.### at ###.#  % Confidence Level"; F#;
       FCONF# * 100
1450 PRINT USING "Standard Deviation of Log(10)P(Torr) =
       ##.###^^^^"; SD#
1460 PRINT USING "Boiling Point = ####.# +/-###.# Celsius";BP;
       BP3
1470 PRINT USING "Variance = ##.###^^^^"; VAR
1480 PRINT USING "Correlation Coefficient = ##.##### "; CORCO
1490 PRINT "Number of Points = "; N
1500 PRINT "Melting Point = "; MP#; "Celsius"
1510 GOSUB 820
```

APPENDIX G

```
1520 PRINT "Comparison of Vapor Pressure of Calculated Values
      with Experimental"
1530 PRINT "            Data for "; COMPOUND$: GOSUB 780
1540 PRINT "Temper- ____Vapor Pressure_____  Differ-"
1550 PRINT " ature  Experimental Calculated   ence
      Method";
1560 PRINT "                Reference"
1570 PRINT "Celsius    Torr        Torr      Percent": GOSUB 780
1580 FOR I = 1 TO N: PRC# = 10# ^ (A# - B# / (C# + T#(I)))
1590 PCD# = (PRC# - G#(I)) * 100# / G#(I)
1600 PRINT USING "###.#   ##.###^^^^  ##.###^^^^"; T#(I); G#(I);
      PRC#;
1610 PRINT USING " ####.##   \                    \ "; PCD#;
      M$(M(I));
1620 PRINT USING " \              \"; C$(I): NEXT I
1630 GOSUB 820
1640 PRINT "Do you want a table of calculated values (Y or N) ";
1650 INPUT Y$
1660 IF Y$ <> "Y" GOTO 1670 ELSE 1680
1670 IF Y$ <> "y" GOTO 2070 ELSE 1680
1680 PRINT "Give lowest, highest, and interval in temperature
      (C)"
1690 PRINT "Low>"; : INPUT L#: PRINT "High>"; : INPUT H#
1700 PRINT "Interval>"; : INPUT INTERVAL#
1710 PRINT "OK (Y or N)>"; : INPUT Y$
1720 IF Y$ = "y" GOTO 1740 ELSE 1730
1730 IF Y$ = "Y" GOTO 1740 ELSE 1650
1740 PRINT CHR$(RPT)
1750 PRINT "                    Calculated Values and Errors":
      PRINT
1760 PRINT "                                  ";
1770 PRINT "     Concentration of"
1780 PRINT "Temperature    Vapor Pressure   ";
1790 PRINT "     Saturated Vapor    Heat of Vaporization"
1800 PRINT "                  _____________________";
1810 PRINT "  ____________________  ____________________"
1820 PRINT "  Celsius    Torr        % Error";
1830 PRINT "   mg/(m cubed)  % Error  cal/mole   % Error": T1# =
      L#: GOSUB 780
1840 C2# = 10 ^ (A# - B# / (C# + T1#)): TK# = T1# + KELVIN#
1850 IF T1# > H# GOTO 1860 ELSE 1870
1860 GOSUB 780: PRINT "* Extrapolated beyond data range.":PRINT :
      GOTO 1630
1870 TPC = T1# + C#: ZX = -1 / TPC: ZSD = SQR(VAR * (1/ N2# + (ZX
      - S1# / N2#) ^ 2 / (S2# - S1# ^ 2 / N2#)))
1880 D3 = C2# * LOG(10) * ZSD
1890 IF (T1# < T#(1)) OR (T1# > T#(N)) GOTO 1900 ELSE 1910
1900 AP$ = "*": GOTO 1920
1910 AP$ = " "
```

APPENDIX G

```
1920 VOL = C2# * MW# / (R# * TK# * 760#) * 1000000#: HEAT = CON#
       * B# * (TK# / TPC) ^ 2
1930 ABCMK = ABS(C# - KELVIN#): SF# = SQR(3# * F#)
1940 SIGHP = (2 * RS * (B#) ^ 2 * (TK#) * ABCMK / ((C2#) * TPC^3
       * (A# - LOG(C2#) / BTEN) ^ 2)) ^ 2
1950 SIGHB = (CON# * TK# ^ 2 / (TPC ^ 2)) ^ 2
1960 SIGHC = (-2! * B# * CON# * TK# ^ 2 / TPC ^ 3) ^ 2
1970 SIGH = SQR(SIGHP * D3 ^ 2 + SIGHB * STDEVB ^ 2 + SIGHC * B9#
       ^ 2)
1980 IF (T1# > MP#) AND ((T1# - INTERVAL#) < MP#) GOTO 1990 ELSE
       2010
1990 PRINT "The melting point is "; MP#; "deg. Celsius.";
2000 PRINT "  The above are for supercooled liquid."
2010 PRINT USING "  ####.#\\ ##.##^^^^   +/-#### ";T1#; AP$; C2#;
       D3 * 100 * SF# / C2#;
2020 PRINT USING "   ##.##^^^^    +/-#### "; VOL;D3 * 100 * SF# /
       C2#;
2030 PRINT USING "   ######. +/- #.###";HEAT * 1000; SIGH * SF# *
       100 / HEAT
2040 T1# = T1# + INTERVAL#: GOTO 1840
2050 REM _____ ROUTING MODULE
     _____
2060 PRINT "Sending directions for plotter to file:A:\ANTplt.plt"
2070 PRINT "For a master plot (M), narrow plot (N), stop (S),
       table(T) >";
2080 INPUT Y$: IF Y$ = "S" OR Y$ = "s" GOTO 2090 ELSE 2100
2090 CLOSE #1: PRINT "File #1 closed.  Normal halt": STOP
2100 IF Y$ = "T" OR Y$ = "t" GOTO 1640 ELSE 2110
2110 IF Y$ = "M" OR Y$ = "m" GOTO 2140 ELSE 2120
2120 IF Y$ = "N" OR Y$ = "n" GOTO 2570 ELSE 2070
2130 REM _____ PLOT ALL DATA
     _____
2140 PRINT "MASTER PLOT: Temperature Range: ";T#(1);" to "; T#(N)
2150 PRINT "Enter Temperature Limits in Celsius(lower,upper) >";
2160 INPUT TB, TT: XMIN = -1! / (TB + C#): XMAX = -1! / (TT + C#)
2170 INPUT "Enter number of times error bars should be
       expanded:";BAR
2180 GOSUB 3000: GOSUB 3010: GOSUB 2910: GOSUB 3080
2190 PRINT #1, "SET SYMBOL 4N"
2200 PRINT #1, "SET ORDER X Y DY"
2210 FOR I = 2 TO 24: RTC = XMIN + (XMAX - XMIN) * I / 25!
2220 PCD# = 10# ^ (A# + B# * RTC): SF# = SQR(3 * F#)
2230 ZX = RTC: ZSD = SQR(VAR * (1 / N2# + (ZX - S1# / N2#) ^ 2 /
       (S2# - S1# ^ 2 / N2#)))
2240 D3 = PCD# * LOG(10) * ZSD * BAR
2250 PRINT #1, RTC, PCD#, D3 * SF#: NEXT I
2260 GOSUB 3180
2270 PRINT #1, "SET SYMBOL 9P": PRINT #1, "SET ORDER X Y"
2280 FOR I = 1 TO N: RTC = -1# / (T#(I) + C#): PRINT #1, RTC,
       G#(I): NEXT I
```

APPENDIX G

```
2290 PRINT #1, "PLOT": GOSUB 2930: GOSUB 2940
2300 REM _____ Celsius Axis
     ____________________________
2310 FOR J = 1 TO 20: TCC = (J - 1) * 10 + TB
2320 IF J > 5 GOTO 2330 ELSE 2340
2330 TCC = (J - 5) * 25 + TB + 50
2340 RTC = -1 / (TCC + C#)
2350 DIST = 2 + 8 * (RTC - XMIN) / (XMAX - XMIN)
2360 IF DIST < 2 GOTO 2420 ELSE 2370
2370 IF DIST > 10 GOTO 2420 ELSE 2380
2380 PRINT #1, USING "LEGEND ##.##### 0.80 JUSTIFY CENTER '";
DIST;
2390 PRINT #1, TCC; "'"
2400 PRINT #1, USING "LEGEND ##.##### 1.12 JUSTIFY CENTER '|'";
       DIST
2410 PRINT #1, "CASE                                        'S'"
2420 NEXT J
2430 GOSUB 2830
2440 REM
```

```
2450 PRINT #1, "LEGEND 2.5 4.9 SIZE=2 'Error bars are";
2460 PRINT #1, BAR; "times'"
2470 PRINT #1, "LEGEND 2.5 4.7 SIZE=2 '  actual limits.'"
2480 RTC = -1 / (BP + C#)
2490 DIST = 2 + 8 * (RTC - XMIN) / (XMAX - XMIN)
2500 PRINT #1, USING "LEGEND ##.##### 2.60 JUSTIFY RIGHT ";DIST +
       .3;
2510 PRINT #1, "'BOILING POINT'"
2520 PRINT #1, USING "LEGEND ##.##### 2.30 JUSTIFY CENTER 'D'";
       DIST
2530 PRINT #1, "CASE                                        'A'"
2540 PRINT #1, "NEW PAGE"
2550 GOTO 2070
2560 REM _____ SUBPLOTS
     ____________________________
2570 PRINT "TOTAL PRESSURE RANGE: "; G#(1); " to "; G#(N)
2580 PRINT "SUBPLOT: Enter vapor pressure limits in
       Torr(lower,upper):";
2590 INPUT PB, PT: PRINT "Lowest vapor pressure:",PB, "Highest:",
       PT
2600 RTC = (A# - LOG(PB) / LOG(10)) / B#: TB = 1 / RTC - C#
2610 RTC = (A# - LOG(PT) / LOG(10)) / B#: TT = 1 / RTC - C#
2620 GOSUB 3000: GOSUB 3100
2630 PRINT #1, "SET SYMBOL 4N"
2640 PRINT #1, "SET ORDER X Y DY"
```

```
2650 FOR I = 1 TO 50: TCC = TB + (TT - TB) * I / 50!
2660 RTC = 1# / (TCC + C#): PCD# = 10# ^ (A# - B# * RTC): SF# =
       SQR(3 * F#)
2670 TPC = TCC + C#: ZX = -1 / TPC
2680 ZSD = SQR(VAR * (1 / N2# + (ZX - S1# / N2#) ^ 2 / (S2# - S1#
       ^ 2 / N2#)))
2690 D3 = PCD# * LOG(10) * ZSD
2700 PRINT #1, TCC, PCD#, D3 * SF#: NEXT I
2710 GOSUB 3180
2720 PRINT #1, "SET SYMBOL 9P": PRINT #1, "SET ORDER X Y"
2730 FOR I = 1 TO N: IF T#(I) > TB AND T#(I) < TT GOTO 2740 ELSE
       2760
2740 RTC = 1# / (T#(I) + C#): PCD# = 10# ^ (A# - B# * RTC)
2750 PRINT #1, T#(I), PCD#
2760 NEXT I
2770 PRINT #1, "PLOT": GOSUB 2960: GOSUB 2830
2780 PRINT #1, "LEGEND 2.5 4.9 SIZE=2 'Error bars are actual
       limits.'"
2790 PRINT #1, "TITLE BOTTOM 'Temperature (C)'"
2800 PRINT #1, "NEW PAGE"
2810 GOTO 2070
2820 REM ***** Subroutine ***** COMPOUND, ANTOINE CONSTANTS, ETC.
2830 PRINT #1, USING "LEGEND 2.5 7 SIZE=3 'Compound:  \
             \'"; COMPOUND$
2840 PRINT #1, "LEGEND 2.5 6.7 SIZE=2 'Antoine Constants:'"
2850 PRINT #1, USING "LEGEND 3 6.4 SIZE=2 'A = ##.####### '"; A#
2860 PRINT #1, USING "LEGEND 3 6.1 SIZE=2 'B = #####.#### '"; B#
2870 PRINT #1, USING "LEGEND 3 5.8 SIZE=2 'C = ####.### '"; C#
2880 PRINT #1, USING "LEGEND 2.5 5.5 SIZE=2 'Boiling Point =
       ###.# C'"; BP
2890 PRINT #1, USING "LEGEND 2.5 5.2 SIZE=2 'Melting Point =
       ####.# C'"; MP#
2900 RETURN
2910 PRINT #1, "SET SCALE Y LOG": RETURN
2920 REM **** Subroutines ***** Stamps, Legend, Titles, Etc. ****
2930 PRINT #1, "STAMP BOTTOM FILENAME": PRINT #1, "STAMP BOTTOM
       DATE": RETURN
2940 PRINT #1, "LEGEND 6 0.6 SIZE=2 JUSTIFY CENTER
       'Temperature(C)'"
2950 PRINT #1, "LEGEND 6 1.35 SIZE=2 JUSTIFY CENTER
       '-1/[Temperature(C)+C]'"
2960 PRINT #1, "TITLE LEFT 'Vapor Pressure (Torr)'": RETURN
2970 REM ***** Subroutine **** Start listing calculations in plot
       file.
2980 PRINT #1, "PLOT": PRINT #1, "set symbol 4P": RETURN
2990 REM ***** Subroutine ***** WINDOWS *****
```

```
3000 PRINT #1, "SET WINDOW X FROM 2 TO 10, Y FROM 2 TO 7.5": RETURN
3010 PRINT #1, "BOX ULC 6 4 SIZE 3.5 1"
3020 PRINT #1, "LEGEND 6.2 3.1 SYMBOL = 4p 'o'"
3030 PRINT #1, "CASE                       'L'"
3040 PRINT #1, "LEGEND 6.5 3.4 SYMBOL = 9P 'o'"
3050 PRINT #1, "LEGEND 7.1 3.1 'Calculated'"
3060 PRINT #1, "LEGEND 7.1 3.4 'Experimental Points'"
3070 PRINT #1, "LEGEND 6.8 3.7 'LEGEND'": RETURN
3080 PRINT #1, USING "SET LIMITS X FROM ##.###### TO ##.######"; XMIN; XMAX
3090 RETURN
3100 PRINT #1, "BOX ULC 6.3 3.4 SIZE 3.5 1.2"
3110 PRINT #1, "LEGEND 6.5 2.5 SYMBOL = 4p 'o'"
3120 PRINT #1, "CASE                       'L'"
3130 PRINT #1, "LEGEND 6.8 2.8 SYMBOL = 9P 'o'"
3140 PRINT #1, "LEGEND 7.4 2.5 'Calculated'"
3150 PRINT #1, "LEGEND 7.4 2.8 'Experimental Points'"
3160 PRINT #1, "LEGEND 7.1 3.1 'LEGEND'": RETURN
3170 REM ***** Subroutine ***** Plot and join data in file *****
3180 PRINT #1, "JOIN": PRINT #1, "PLOT": RETURN
3190 REM _____ END OF PLOTTING
3200 REM ***** Subroutine ***** Warning of unusual C values *****
3210 IF C# < 200# GOTO 3220 ELSE 3230
3220 PRINT "C is less than 200. C= "; C#: RETURN
3230 IF C# > 273.15# GOTO 3240 ELSE RETURN
3240 PRINT "C is greater than 273.16  C= "; C#: RETURN
3250 REM ***** Subroutine ***** Computation of A, B, and S *****
3260 S1# = 0#: S2# = 0#: S3# = 0#: S4# = 0#: S5# = 0#
3270 FOR K = 1 TO N: X# = (-1#) / (T#(K) + CAA#): YY# = Y#(K)
3280 S4# = S4# + YY#: S5# = S5# + YY# ^ 2
3290 S1# = S1# + X#: S2# = S2# + X# * X#: S3# = S3# + YY# * X#
3300 NEXT K: N2# = CDBL(N)
3310 D# = (N2# * S2# - S1# * S1#)
3320 B# = (N2# * S3# - S1# * S4#) / D#
3330 A# = (S4# - B# * S1#) / N2#
3340 S# = S5# + A# ^ 2# * N2# - 2# * A# * S4# - 2 * B# * S3# + 2# * A# * B# * S1# + B# ^ 2# * S2#
3350 RETURN
3360 REM ***** Subroutine ***** Final Computation *****
3370 S1# = 0#: S2# = 0#: S3# = 0#: S4# = 0#: S5# = 0#: S9# = 0
3380 FOR K = 1 TO N: X# = (-1#) / (T#(K) + C#): YY# = Y#(K)
3390 S4# = S4# + YY#: S5# = S5# + YY# ^ 2
3400 S1# = S1# + X#: S2# = S2# + X# * X#: S3# = S3# + YY# * X#
3410 NEXT K: N2# = CDBL(N)
3420 D# = (N2# * S2# - S1# * S1#)
3430 B# = (N2# * S3# - S1# * S4#) / D#
```

APPENDIX G

```
3440 A# = (S4# - B# * S1#) / N2#
3450 S# = S5# + A# ^ 2# * N2# - 2# * A# * S4# - 2 * B# * S3# + 2#
       * A# * B# * S1# + B# ^ 2# * S2#
3460 FOR K = 1 TO N: S9# = S9# + (Y#(K) - S4# / N2#) ^ 2: NEXT K
3470 VAR = S# / (N2# - 2#): STDEVB = SQR(N2# * VAR / D#)
3480 CORCO = SQR(1 - S# / S9#): STDEVA = SQR(VAR * (1!+ S1# ^ 2 /
       (D# * N2#)))
3490 RETURN
3500 REM ***** Subroutine ***** F-Distribution *****
3510 REM      Calculates F from confidence level and N, the
       number of points
3520 DIM Z#(10): PRINT "This part is slow.  Keep smiling. THE
       COMPUTER'S OK.  ";
3530 PI# = 3.141593#: V# = CDBL(N - 3)
3540 IF V# < 2# GOTO 3730 ELSE 3550
3550 U# = 3#: UV# = (U# + V#)/2#: ARG# = UV#: NIT = 10000: FF# =
       0#: PNIT = 500
3560 GOSUB 3750
3570 Z#(1) = LOGGAMMA#: U2# = U# / 2#: ARG# = U2#
3580 GOSUB 3750
3590 Z#(2) = LOGGAMMA#: ARG# = V# / 2#
3600 GOSUB 3750
3610 Z#(3) = LOGGAMMA#: XX# = Z#(1) - Z#(2) - Z#(3)
3620 FX# = XX# + (U# / 2#) * LOG(U#) + (V# / 2#) * LOG(V#)
3630 FOR ITER = 1 TO NIT: E = ITER * 20 / NIT: F# = CDBL(E)
3640 REM ***** Holding Printer ******
3650 IF ITER = PNIT GOTO 3660 ELSE 3670
3660 PRINT CHR$(1); : PNIT = 100 + PNIT
3670 GX# = FX# + LOG(F#) * (U2# - 1#) - LOG(V# + F# * U#) * UV#:
       GX# = EXP(GX#)
3680 FF# = FF# + GX# * CDBL(20 / NIT)
3690 IF FF# > FCONF# GOTO 3720 ELSE 3700
3700 NEXT ITER
3710 PRINT "PROBLEM **** F exceeds 20 **** ": STOP
3720 RETURN
3730 PRINT "PROBLEM: Degrees of Freedom Less than 2 ";FCONF#, V#:
       STOP
3740 REM ***** Subroutine ***** F-Distribution *****
3750 L2# = -1# / (360# * ARG# ^ 3#) + 1# /(1260# * ARG# ^5#) - 1#
       / (1680# * ARG# ^ 7#)
3760 L1# = (ARG# - .5#) * LOG(ARG#) - ARG# + .5# * LOG(2#*PI#) +
       1# / (12# * ARG#) + L2#
3770 LOGGAMMA# = L1#: RETURN
```

```
3780 REM  *****DATA *****
4000 DATA "C7H12O4",3,66,"C",7,"H",12,"O",4, "Diethyl
      Malonate",-48.9
4010 DATA  -8,0.011,"89BRO/FIE",3
4020 DATA  -5.5,0.014,"89BRO/FIE",3
4030 DATA  -4.1,0.015,"89BRO/FIE",3
4040 DATA  -2.6,0.018,"89BRO/FIE",3
4050 DATA  -1.5,0.019,"89BRO/FIE",3
4060 DATA  -0.3,0.025,"89BRO/FIE",3
4070 DATA   1.0,0.025,"89BRO/FIE",3
4080 DATA   2.5,0.033,"89BRO/FIE",3
4090 DATA   3.6,0.033,"89BRO/FIE",3
4100 DATA   4.7,0.041,"89BRO/FIE",3
4110 DATA   6.7,0.048,"89BRO/FIE",3
4120 DATA   9.7,0.060,"89BRO/FIE",3
4130 DATA  11.4,0.069,"89BRO/FIE",3
4140 DATA  14.8,0.092,"89BRO/FIE",3
4150 DATA  64.2,3.1 ,"89BRO/FIE",8
4160 DATA  64.6,3.2 ,"89BRO/FIE",8
4170 DATA  66.5,3.6 ,"89BRO/FIE",8
4180 DATA  70.8,4.7 ,"89BRO/FIE",8
4190 DATA  72.9,5.3 ,"89BRO/FIE",8
4200 DATA  74.6,5.9 ,"89BRO/FIE",8
4210 DATA  75.4,6.3 ,"89BRO/FIE",8
4220 DATA  76.9,6.7 ,"89BRO/FIE",8
4230 DATA  78.0,7.5 ,"89BRO/FIE",8
4240 DATA  78.5,7.4 ,"89BRO/FIE",8
4250 DATA  78.7,7.5 ,"89BRO/FIE",8
4260 DATA  79.2,7.5 ,"89BRO/FIE",8
4270 DATA  79.4,8.0 ,"89BRO/FIE",8
4280 DATA  80.5,8.4 ,"89BRO/FIE",8
4290 DATA  80.6,8.6 ,"89BRO/FIE",8
4300 DATA  81.7,9.2 ,"89BRO/FIE",8
4310 DATA  81.8,9.7 ,"89BRO/FIE",8
4320 DATA  83.6,10.1 ,"89BRO/FIE",8
4330 DATA  83.8,10.4 ,"89BRO/FIE",8
4340 DATA  85.9,12.1 ,"89BRO/FIE",8
4350 DATA  88.0,13.2 ,"89BRO/FIE",8
4360 DATA  90.2,15.1 ,"89BRO/FIE",8
4370 DATA  92.9,17.0 ,"89BRO/FIE",8
4380 DATA  97.0,20.5 ,"89BRO/FIE",8
4390 DATA 101.2,25.1 ,"89BRO/FIE",8
4400 DATA 105.3,30.3 ,"89BRO/FIE",8
```

```
4410 DATA 111.1,39.5 ,"89BRO/FIE",8
4420 DATA 116.6,49.8 ,"89BRO/FIE",8
4430 DATA 121.2,60.0 ,"89BRO/FIE",8
4440 DATA 124.5,69.3 ,"89BRO/FIE",8
4450 DATA 128.3,80.3 ,"89BRO/FIE",8
4460 DATA 131.0,89.8 ,"89BRO/FIE",8
4470 DATA 133.2,97.8 ,"89BRO/FIE",8
4480 DATA 138.5,117.4 ,"89BRO/FIE",8
4490 DATA 143.0,139.0,"89BRO/FIE",8
4500 DATA 148.8,169.9,"89BRO/FIE",8
4510 DATA 153.9,200.4,"89BRO/FIE",8
4520 DATA 160.2,250.4 ,"89BRO/FIE",8
4530 DATA 165.9,300.2 ,"89BRO/FIE",8
4540 DATA 170.0,338.2,"89BRO/FIE",8
4550 DATA 174.7,396.8 ,"89BRO/FIE",8
4560 DATA 178.9,450.2,"89BRO/FIE",8
4570 DATA 182.5,502.0,"89BRO/FIE",8
4580 DATA 189.0,599.8,"89BRO/FIE",8
4590 DATA 190.0,659.6,"89BRO/FIE",8
4600 DATA 192.4,660.3,"89BRO/FIE",8
4610 DATA 195.9,756.1,"89BRO/FIE",8
4620 DATA 196.2,761.4,"89BRO/FIE",8
4630 DATA 197.1,775.4,"89BRO/FIE",8
4640 DATA 197.3,781.7,"89BRO/FIE",8
4650 DATA 197.5,775.1,"89BRO/FIE",8
4660 DATA 198.1,781.2,"89BRO/FIE",8
```

APPENDIX G

APPENDIX H

DATA INPUT FORMAT

Line 4000 of Appendix G is the first line of a sample data input. It is recommended that data points be entered in ler from low to high temperature. Data points must be stored a basic file starting with line 4000. Save the file with the ' option (SAVE "DATAFILE.BAS",A). To merge with the program ıd the program (LOAD "ANT592.BAS"), and merge with the data le (MERGE "DATAFILE.BAS"). If the data file is not saved with) "A" option, merging will not be possible. The data is tered into a basic file to preserve the full screen editing pabilities of GW BASIC or QBASIC.

Data is entered in the following order separated by mmas:

ımental formula in quotes,
ıber of elements in compound,
ıber of data points,
rst element symbol in quotes,
ıber of atoms of first element,
:ond element symbol in quotes,
ıber of atoms of second element,

.

mpound name in quotes,
ezing point in Celsius,

<u>irst data point)</u>
mperature(Celsius), Vapor Pressure (Torr), Reference Code*,
ıber for Experimental Method**,

See Appendix E.
See Table 4 in section 3.5 of the report.

{Second data point}
Temperature(Celsius), Vapor Pressure (Torr), Reference Code*,
Number for Experimental Method**,

...
...

{N-th data point}
Temperature(Celsius), Vapor Pressure (Torr), Reference Code*,
Number for Experimental Method**,

---

* See Appendix E.
** See Table 4 in section 3.5 of the report.

APPENDIX H

APPENDIX I

SAMPLE COMPUTER RUN

```
run
ADVANCED VAPOR PRESSURE DATA ANALYSIS AND PLOTTING

  PROGRAM: ANT592.BAS
Run date is 06-06-1992
Is 95% confidence level OK? (Y or N) ? y
The  95.0 % confidence level was chosen.
Do you intend to plot? (Y or N) ? n
```

Element	Atomic Weight	Number	Experimental Method
C	12.01100	1	Isoteniscope
H	1.00790	2	Boiling Point
Br	79.90400	3	Effusion
Cl	35.45300	4	Dynamic Gas Saturation
F	18.99840	5	Manometer
N	14.00670	6	Tensimeter
O	15.99940	7	Gas Chromatography
P	30.97380	8	DTA
S	32.06000	9	Ebulliometry
Si	28.08600	10	Calculated
	0.00000	11	Method Not Given
	0.00000	12	Droplet Evaporation

```
Elemental Formula = C7H12O4      C 7 H 12 O 4
Calculated Molecular Weight of Diethyl Malonate =  160.1694

Hit Enter or Return Key?
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Experimental Data, Methods, and References for Diethyl Malonate

Temperature Celsius	Vapor Pressure Torr	Reference	Method
-8.0	1.100D-02	89BRO/FIE	Effusion
-5.5	1.400D-02	89BRO/FIE	Effusion
-4.1	1.500D-02	89BRO/FIE	Effusion
-2.6	1.800D-02	89BRO/FIE	Effusion
-1.5	1.900D-02	89BRO/FIE	Effusion
-0.3	2.500D-02	89BRO/FIE	Effusion
1.0	2.500D-02	89BRO/FIE	Effusion
2.5	3.300D-02	89BRO/FIE	Effusion
3.6	3.300D-02	89BRO/FIE	Effusion
4.7	4.100D-02	89BRO/FIE	Effusion
6.7	4.800D-02	89BRO/FIE	Effusion
9.7	6.000D-02	89BRO/FIE	Effusion
11.4	6.900D-02	89BRO/FIE	Effusion
14.8	9.200D-02	89BRO/FIE	Effusion
64.2	3.100D+00	89BRO/FIE	DTA
64.6	3.200D+00	89BRO/FIE	DTA
66.5	3.600D+00	89BRO/FIE	DTA
70.8	4.700D+00	89BRO/FIE	DTA
72.9	5.300D+00	89BRO/FIE	DTA
74.6	5.900D+00	89BRO/FIE	DTA
75.4	6.300D+00	89BRO/FIE	DTA
76.9	6.700D+00	89BRO/FIE	DTA
78.0	7.500D+00	89BRO/FIE	DTA
78.5	7.400D+00	89BRO/FIE	DTA
78.7	7.500D+00	89BRO/FIE	DTA
79.2	7.500D+00	89BRO/FIE	DTA
79.4	8.000D+00	89BRO/FIE	DTA
80.5	8.400D+00	89BRO/FIE	DTA
80.6	8.600D+00	89BRO/FIE	DTA
81.7	9.200D+00	89BRO/FIE	DTA
81.8	9.700D+00	89BRO/FIE	DTA
83.6	1.010D+01	89BRO/FIE	DTA
83.8	1.040D+01	89BRO/FIE	DTA
85.9	1.210D+01	89BRO/FIE	DTA
88.0	1.320D+01	89BRO/FIE	DTA
90.2	1.510D+01	89BRO/FIE	DTA
92.9	1.700D+01	89BRO/FIE	DTA
97.0	2.050D+01	89BRO/FIE	DTA
10[illegible].2	2.510D+01	89BRO/FIE	DTA
105.3	3.030D+01	89BRO/FIE	DTA

111.1	3.950D+01	89BRO/FIE	DTA
116.6	4.980D+01	89BRO/FIE	DTA
121.2	6.000D+01	89BRO/FIE	DTA
124.5	6.930D+01	89BRO/FIE	DTA
128.3	8.030D+01	89BRO/FIE	DTA
131.0	8.980D+01	89BRO/FIE	DTA
133.2	9.780D+01	89BRO/FIE	DTA
138.5	1.174D+02	89BRO/FIE	DTA
143.0	1.390D+02	89BRO/FIE	DTA
148.8	1.699D+02	89BRO/FIE	DTA
153.9	2.004D+02	89BRO/FIE	DTA
160.2	2.504D+02	89BRO/FIE	DTA
165.9	3.002D+02	89BRO/FIE	DTA
170.0	3.382D+02	89BRO/FIE	DTA
174.7	3.968D+02	89BRO/FIE	DTA
178.9	4.502D+02	89BRO/FIE	DTA
182.5	5.020D+02	89BRO/FIE	DTA
189.0	5.998D+02	89BRO/FIE	DTA
190.0	6.596D+02	89BRO/FIE	DTA
192.4	6.603D+02	89BRO/FIE	DTA
195.9	7.561D+02	89BRO/FIE	DTA
196.2	7.614D+02	89BRO/FIE	DTA
197.1	7.754D+02	89BRO/FIE	DTA
197.3	7.817D+02	89BRO/FIE	DTA
197.5	7.751D+02	89BRO/FIE	DTA
198.1	7.812D+02	89BRO/FIE	DTA

**********EVALUATE 55 C's FOR MAXIMUMS AND MINIMUMS*********
This is helpful only with a narrow temp. range or poor data.

C	S	C	S	C	S
50.0	10.8298163595907	60.0	8.2026595811847	70.0	6.2676915851207
80.0	4.8064222984003	90.0	3.6856454330643	100.0	2.8174990348730
110.0	2.1410028376933	120.0	1.6123246359224	130.0	1.1991425925279
140.0	0.8771505780394	150.0	0.6277812709345	160.0	0.4366660383680
170.0	0.2925625363267	180.0	0.1865905340635	190.0	0.1116769697460
200.0	0.0621464941121	210.0	0.0334152143457	220.0	0.0217588859371
230.0	0.0241355963905	240.0	0.0380488442436	250.0	0.0614409033073
260.0	0.0926091235237	270.0	0.1301397631736	280.0	0.1728553338492
290.0	0.2197724414173	300.0	0.2700678380853	310.0	0.3230509407939
320.0	0.3781414735020	330.0	0.4348511931806	340.0	0.4927688882170
350.0	0.5515480125622	360.0	0.6108964530489	370.0	0.6705680310174
380.0	0.7303554200648	390.0	0.7900842248002	400.0	0.8496080151851
410.0	0.9088041502223	420.0	0.9675702559973	430.0	1.0258212479387
440.0	1.0834868071720	450.0	1.1405092368386	460.0	1.1968416373359
470.0	1.2524463499335	480.0	1.3072936268341	490.0	1.3613604927359
500.0	1.4146297688085	510.0	1.4670892346212	520.0	1.5187309076018
530.0	1.5695504227133	540.0	1.6195464978832	550.0	1.6687204728221
560.0	1.7170759108608	570.0	1.7646182548995	580.0	1.8113545299743
590.0	1.8572930859973				

C for minimum S = 220
Minimum S = 2.175888593706077D-02
Number of minimums = 1

********** FINE TUNING OF C **********
220.000 225.250 222.625 222.625 223.281 222.953 223.117 223.117 223.076
223.076 223.081 223.081 223.081 223.081 223.081

Review of Fitting Process

Final C = 223.0810 at an Interval of 0.00135
Final S = 0.0211210814095 after 16 th step
Number of digits required in calculation is 12

RESULTS

Antoine Constants for Diethyl Malonate:
A = 8.0005804 B = 2146.40052 C = 223.081

Standard Deviation of A = 0.020955 and of B = 3.200
F = 2.752 at 95.0 % Confidence Level
Standard Deviation of Log(10)P(Torr) = 1.817D-02
Boiling Point = 196.2 +/- 0.8 Celsius
Variance = 3.300E-04
Correlation Coefficient = 0.99993
Number of Points = 66
Melting Point = -48.9 Celsius

Hit Enter or Return Key?

APPENDIX I

Comparison of Vapor Pressure of Calculated Values with Experimental Data for Diethyl Malonate

Temperature Celsius	Vapor Pressure Experimental Torr	Vapor Pressure Calculated Torr	Difference Percent	Method	Reference
-8.0	1.100D-02	1.050D-02	-4.57	Effusion	89BRO/FIE
-5.5	1.400D-02	1.367D-02	-2.36	Effusion	89BRO/FIE
-4.1	1.500D-02	1.581D-02	5.37	Effusion	89BRO/FIE
-2.6	1.800D-02	1.843D-02	2.38	Effusion	89BRO/FIE
-1.5	1.900D-02	2.060D-02	8.41	Effusion	89BRO/FIE
-0.3	2.500D-02	2.323D-02	-7.09	Effusion	89BRO/FIE
1.0	2.500D-02	2.642D-02	5.67	Effusion	89BRO/FIE
2.5	3.300D-02	3.059D-02	-7.30	Effusion	89BRO/FIE
3.6	3.300D-02	3.402D-02	3.10	Effusion	89BRO/FIE
4.7	4.100D-02	3.780D-02	-7.81	Effusion	89BRO/FIE
6.7	4.800D-02	4.566D-02	-4.88	Effusion	89BRO/FIE
9.7	6.000D-02	6.024D-02	0.40	Effusion	89BRO/FIE
11.4	6.900D-02	7.027D-02	1.83	Effusion	89BRO/FIE
14.8	9.200D-02	9.497D-02	3.23	Effusion	89BRO/FIE
64.2	3.100D+00	3.382D+00	9.09	DTA	89BRO/FIE
64.6	3.200D+00	3.464D+00	8.24	DTA	89BRO/FIE
66.5	3.600D+00	3.877D+00	7.69	DTA	89BRO/FIE
70.8	4.700D+00	4.977D+00	5.89	DTA	89BRO/FIE
72.9	5.300D+00	5.607D+00	5.80	DTA	89BRO/FIE
74.6	5.900D+00	6.168D+00	4.55	DTA	89BRO/FIE
75.4	6.300D+00	6.449D+00	2.37	DTA	89BRO/FIE
76.9	6.700D+00	7.006D+00	4.56	DTA	89BRO/FIE
78.0	7.500D+00	7.440D+00	-0.79	DTA	89BRO/FIE
78.5	7.400D+00	7.646D+00	3.32	DTA	89BRO/FIE
78.7	7.500D+00	7.729D+00	3.06	DTA	89BRO/FIE
79.2	7.500D+00	7.941D+00	5.89	DTA	89BRO/FIE
79.4	8.000D+00	8.028D+00	0.35	DTA	89BRO/FIE
80.5	8.400D+00	8.517D+00	1.40	DTA	89BRO/FIE
80.6	8.600D+00	8.563D+00	-0.43	DTA	89BRO/FIE
81.7	9.200D+00	9.081D+00	-1.29	DTA	89BRO/FIE
81.8	9.700D+00	9.130D+00	-5.88	DTA	89BRO/FIE
83.6	1.010D+01	1.004D+01	-0.58	DTA	89BRO/FIE
83.8	1.040D+01	1.015D+01	-2.43	DTA	89BRO/FIE
85.9	1.210D+01	1.132D+01	-6.44	DTA	89BRO/FIE
88.0	1.320D+01	1.261D+01	-4.46	DTA	89BRO/FIE
90.2	1.510D+01	1.410D+01	-6.62	DTA	89BRO/FIE
92.9	1.700D+01	1.613D+01	-5.09	DTA	89BRO/FIE
97.0	2.050D+01	1.971D+01	-3.83	DTA	89BRO/FIE
101.2	2.510D+01	2.408D+01	-4.07	DTA	89BRO/FIE
105.3	3.030D+01	2.913D+01	-3.88	DTA	89BRO/FIE
111.1	3.950D+01	3.782D+01	-4.26	DTA	89BRO/FIE
116.6	4.980D+01	4.805D+01	-3.51	DTA	89BRO/FIE
121.2	6.000D+01	5.836D+01	-2.73	DTA	89BRO/FIE
124.5	6.930D+01	6.688D+01	-3.49	DTA	89BRO/FIE
128.3	8.030D+01	7.800D+01	-2.86	DTA	89BRO/FIE
131.0	8.980D+01	8.683D+01	-3.30	DTA	89BRO/FIE
133.2	9.780D+01	9.465D+01	-3.22	DTA	89BRO/FIE
138.5	1.174D+02	1.160D+02	-1.20	DTA	89BRO/FIE
143.0	1.390D+02	1.372D+02	-1.29	DTA	89BRO/FIE
148.8	1.699D+02	1.694D+02	-0.31	DTA	89BRO/FIE

153.9	2.004D+02	2.027D+02	1.16	DTA	89BRO/FIE
160.2	2.504D+02	2.515D+02	0.43	DTA	89BRO/FIE
165.9	3.002D+02	3.038D+02	1.20	DTA	89BRO/FIE
170.0	3.382D+02	3.468D+02	2.55	DTA	89BRO/FIE
174.7	3.968D+02	4.024D+02	1.41	DTA	89BRO/FIE
178.9	4.502D+02	4.582D+02	1.77	DTA	89BRO/FIE
182.5	5.020D+02	5.110D+02	1.79	DTA	89BRO/FIE
189.0	5.998D+02	6.193D+02	3.25	DTA	89BRO/FIE
190.0	6.596D+02	6.375D+02	-3.35	DTA	89BRO/FIE
192.4	6.603D+02	6.832D+02	3.46	DTA	89BRO/FIE
195.9	7.561D+02	7.545D+02	-0.21	DTA	89BRO/FIE
196.2	7.614D+02	7.609D+02	-0.06	DTA	89BRO/FIE
197.1	7.754D+02	7.804D+02	0.64	DTA	89BRO/FIE
197.3	7.817D+02	7.848D+02	0.39	DTA	89BRO/FIE
197.5	7.751D+02	7.892D+02	1.81	DTA	89BRO/FIE
198.1	7.812D+02	8.025D+02	2.72	DTA	89BRO/FIE

Hit Enter or Return Key?

APPENDIX I

Calculated Values and Estimated Error Limits for Diethyl Malonate

Temperature	Vapor Pressure		Concentration of Saturated Vapor		Heat of Vaporization	
Celsius	Torr	% Error	mg/(m cubed)	% Error	cal/mole	% Error
0.0	2.39D-02	+/- 3	2.25E+02	+/- 3	14725.	+/- 0.431
1.0	2.64D-02	+/- 3	2.48E+02	+/- 3	14701.	+/- 0.431
2.0	2.91D-02	+/- 3	2.72E+02	+/- 3	14677.	+/- 0.431
3.0	3.21D-02	+/- 3	2.99E+02	+/- 3	14653.	+/- 0.431
4.0	3.54D-02	+/- 3	3.28E+02	+/- 3	14630.	+/- 0.431
5.0	3.89D-02	+/- 3	3.59E+02	+/- 3	14607.	+/- 0.431
6.0	4.28D-02	+/- 3	3.93E+02	+/- 3	14584.	+/- 0.431
7.0	4.70D-02	+/- 3	4.30E+02	+/- 3	14561.	+/- 0.431
8.0	5.15D-02	+/- 3	4.71E+02	+/- 3	14538.	+/- 0.431
9.0	5.65D-02	+/- 3	5.14E+02	+/- 3	14516.	+/- 0.431
10.0	6.19D-02	+/- 3	5.62E+02	+/- 3	14494.	+/- 0.431
11.0	6.78D-02	+/- 3	6.13E+02	+/- 3	14472.	+/- 0.431
12.0	7.41D-02	+/- 3	6.68E+02	+/- 3	14450.	+/- 0.430
13.0	8.11D-02	+/- 3	7.28E+02	+/- 3	14429.	+/- 0.430
14.0	8.85D-02	+/- 3	7.92E+02	+/- 3	14408.	+/- 0.430
15.0	9.66D-02	+/- 2	8.61E+02	+/- 2	14387.	+/- 0.430
16.0	1.05D-01	+/- 2	9.36E+02	+/- 2	14366.	+/- 0.430
17.0	1.15D-01	+/- 2	1.02E+03	+/- 2	14345.	+/- 0.430
18.0	1.25D-01	+/- 2	1.10E+03	+/- 2	14324.	+/- 0.430
19.0	1.36D-01	+/- 2	1.20E+03	+/- 2	14304.	+/- 0.430
20.0	1.48D-01	+/- 2	1.30E+03	+/- 2	14284.	+/- 0.430
21.0	1.61D-01	+/- 2	1.41E+03	+/- 2	14264.	+/- 0.430
22.0	1.75D-01	+/- 2	1.52E+03	+/- 2	14244.	+/- 0.430
23.0	1.90D-01	+/- 2	1.65E+03	+/- 2	14224.	+/- 0.430
24.0	2.06D-01	+/- 2	1.78E+03	+/- 2	14205.	+/- 0.430
25.0	2.23D-01	+/- 2	1.92E+03	+/- 2	14186.	+/- 0.430
26.0	2.42D-01	+/- 2	2.08E+03	+/- 2	14167.	+/- 0.430
27.0	2.62D-01	+/- 2	2.24E+03	+/- 2	14148.	+/- 0.430
28.0	2.83D-01	+/- 2	2.41E+03	+/- 2	14129.	+/- 0.430
29.0	3.06D-01	+/- 2	2.60E+03	+/- 2	14110.	+/- 0.430
30.0	3.31D-01	+/- 2	2.80E+03	+/- 2	14092.	+/- 0.430
31.0	3.57D-01	+/- 2	3.02E+03	+/- 2	14073.	+/- 0.430
32.0	3.85D-01	+/- 2	3.24E+03	+/- 2	14055.	+/- 0.430
33.0	4.16D-01	+/- 2	3.49E+03	+/- 2	14037.	+/- 0.430
34.0	4.48D-01	+/- 2	3.75E+03	+/- 2	14019.	+/- 0.430
35.0	4.83D-01	+/- 2	4.02E+03	+/- 2	14002.	+/- 0.430
36.0	5.20D-01	+/- 2	4.32E+03	+/- 2	13984.	+/- 0.430
37.0	5.59D-01	+/- 2	4.63E+03	+/- 2	13967.	+/- 0.430
38.0	6.02D-01	+/- 2	4.97E+03	+/- 2	13949.	+/- 0.430
39.0	6.47D-01	+/- 2	5.32E+03	+/- 2	13932.	+/- 0.430
40.0	6.95D-01	+/- 2	5.70E+03	+/- 2	13915.	+/- 0.430

* Extrapolated beyond data range.

APPENDIX I

Calculated Values and Estimated Error Limits for Diethyl Malonate

Temperature	Vapor Pressure			Concentration of Saturated Vapor			Heat of Vaporization		
Celsius	Torr	%	Error	mg/(m cubed)	%	Error	cal/mole	%	Error
-140.0*	1.46D-18	+/-	19	2.82E-14	+/-	19	25226.	+/-	0.489
-120.0*	1.51D-13	+/-	14	2.53E-09	+/-	14	21679.	+/-	0.467
-100.0*	3.64D-10	+/-	10	5.41E-06	+/-	10	19437.	+/-	0.454
-80.0*	9.98D-08	+/-	8	1.33E-03	+/-	8	17898.	+/-	0.445
-60.0*	6.90D-06	+/-	6	8.32E-02	+/-	6	16778.	+/-	0.439
The melting point is -48.9 deg. Celsius. The above are for supercooled liquid.									
-40.0*	1.89D-04	+/-	5	2.08E+00	+/-	5	15928.	+/-	0.435
-20.0*	2.70D-03	+/-	4	2.74E+01	+/-	4	15261.	+/-	0.433
0.0	2.39D-02	+/-	3	2.25E+02	+/-	3	14725.	+/-	0.431
20.0	1.48D-01	+/-	2	1.30E+03	+/-	2	14284.	+/-	0.430
40.0	6.95D-01	+/-	2	5.70E+03	+/-	2	13915.	+/-	0.430
60.0	2.62D+00	+/-	2	2.02E+04	+/-	2	13603.	+/-	0.429
80.0	8.29D+00	+/-	1	6.03E+04	+/-	1	13334.	+/-	0.429
100.0	2.28D+01	+/-	2	1.57E+05	+/-	2	13101.	+/-	0.429
120.0	5.55D+01	+/-	2	3.53E+05	+/-	2	12897.	+/-	0.429
140.0	1.23D+02	+/-	2	7.63E+05	+/-	2	12717.	+/-	0.430
160.0	2.50D+02	+/-	2	1.48E+06	+/-	2	12556.	+/-	0.430
180.0	4.74D+02	+/-	2	2.69E+06	+/-	2	12413.	+/-	0.430
200.0*	8.46D+02	+/-	2	4.59E+06	+/-	2	12283.	+/-	0.431
220.0*	1.43D+03	+/-	3	7.46E+06	+/-	3	12166.	+/-	0.431
240.0*	2.32D+03	+/-	3	1.16E+07	+/-	3	12060.	+/-	0.431
260.0*	3.61D+03	+/-	3	1.74E+07	+/-	3	11963.	+/-	0.432
280.0*	5.42D+03	+/-	3	2.52E+07	+/-	3	11873.	+/-	0.432
300.0*	7.89D+03	+/-	3	3.54E+07	+/-	3	11791.	+/-	0.432

* Extrapolated beyond data range.

END

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DATE: 9-92

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